

Genetic Algorithms as Global Random Search Methods

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Abstract

Genetic algorithm behavior is described in terms of the construction and evolution of the sampling distributions over the space of candidate solutions. This novel perspective is motivated by analysis indicating that the schema theory is inadequate for completely and properly explaining genetic algorithm behavior. Based on the proposed theory, it is argued that the similarities of candidate solutions should be exploited directly, rather than encoding candidate solutions and then exploiting their similarities. Proportional selection is characterized as a global search operator, and recombination is characterized as the search process that exploits similarities. Sequential algorithms and many deletion methods are also analyzed. It is shown that by properly constraining the search breadth of recombination operators, convergence of genetic algorithms to a global optimum can be ensured.

1 Introduction

Genetic algorithms are adaptive systems designed to emulate natural evolution. They were first proposed by John Holland in 1975 in his seminal work *Adaptation in Natural and Artificial Systems* (Holland, 1975). De Jong suggests that genetic algorithms should be understood from the perspectives of genotypic and phenotypic behavior, as well as their performance as global optimizers (De Jong, 1993). This paper contributes to this goal by describing genetic algorithm behavior in terms of the sampling distributions they impose on the genospace and the phenospace, and how these distributions contribute to or detract from the optimization process.

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While genetic algorithms have been shown to be effective in many problem domains, the theoretical foundation for describing, explaining, and predicting their behavior is presently inadequate. As argued in Section 2, the prevailing theory of genetic algorithm behavior, the schema theory, is not a suitable theory for describing genetic algorithm behavior. Accordingly, the primary objective of this paper is to generalize genetic algorithms and to provide an adequate basis for their understanding and analysis (Sections 3 & 4). A second objective of this paper is to explore the issues and variations of genetic algorithms permitted by their generalization in the context of the proposed explanation of genetic algorithm behavior (Section 5). The final objective of this paper is to determine the conditions under which genetic algorithms can be assured to converge to a global optimum (Section 6). Finally, conclusions and suggestions for future research are presented (Section 7).

2 Descriptions and Analyses of Genetic Algorithm Behavior

In this section, descriptions and analyses of genetic algorithm behavior are considered. Naturally, the most basic description of a genetic algorithm and the fundamental basis of analysis is its definition. For the purposes of this paper, the canonical genetic algorithm is defined by Procedure 1. In step 3 and throughout the paper, the *recombination* of parental encodings is taken to include the effects of both mutation and crossover. Common recombination operators and fitness scaling techniques are described throughout the literature (general coverage is provided in (Holland, 1975; Goldberg, 1989a; Davis, 1991)). In subsection 2.1, where the schema theory is considered, it is assumed that no fitness scaling is used and that the entire population of chromosomes is replaced each generation.

Procedure 1 The Canonical Genetic Algorithm

1. Initialize a population of chromosomes (binary strings).

2. Evaluate each chromosome in the population by applying the objective function to its corresponding candidate solution.
3. Create new chromosomes by applying a fitness scaling technique to the chromosome evaluations, choosing parent chromosomes according to their relative fitness, and recombining their encodings.
4. Delete members of the population to make room for the new chromosomes.
5. Evaluate each new chromosome as in Step 2, and insert it into the population.
6. If the stopping criterion has been satisfied, then stop and return the chromosome with the best observed fitness; otherwise continue with Step 3.

While the procedural description is complete and exact, it is not adequate for conveying a suitable understanding of genetic algorithm behavior. This description is able to explain phenomena arising from the use of a genetic algorithm only at the lowest level of abstraction and understanding. Since this description operates at the experimental, practical, or phenomenal level, it does not constitute a theory. Consequently, the inadequacies of this description have given rise to the schema theory and other analyses of genetic algorithms, such as Markov chain analysis.

In the remainder of this section, the suitability of existing analyses of genetic algorithm behavior are considered on the basis of the following criteria:

1. The theory should be well grounded in the procedural elements and the generating mechanisms of genetic algorithms. These include the processes of selection, recombination, fitness evaluation, and population management.
2. The theory should have explanatory and predictive power.
3. The theory should be robust with respect to algorithmic variations.

Furthermore, in consideration of Occam's razor, the preferred theory is the simplest and most closely grounded to that which is known (*i.e.*, the procedural elements and generating mechanisms).

In this paper, an individual string is denoted A or A_j , where $j = 1, 2, \dots, N$, and N is the size of the population $\mathbf{A}(t)$ at time t . The objective or fitness function is denoted $f : \mathcal{A} \rightarrow \mathbb{R}^1 > 0$. A schema, its *order*, and its *defining length*, are denoted H , $o(H)$, and $\delta(H)$, respectively. A schema's order is the number of fixed positions or string elements common to all members of the schema, and its defining length is the distance between the schema's first and last fixed positions.

2.1 The Schema Theory

According to the schema theory, genetic algorithms work in the space of schemata as opposed to the space of strings. Therefore, it is necessary to understand the effects of reproduction and the recombination operators on the schemata contained within a population in order to understand the behavior of genetic algorithms within the context of the schema theory. When proportional selection is used, the probability of selecting $A_{j,t}$, the j th individual in the population at time t , as a parent is

$$p_{j,t} = \frac{f(A_{j,t})}{\sum_{A_{i,t} \in \mathbf{A}(t)} f(A_{i,t})}, \quad (1)$$

and, the target sampling rate of a schema H is

$$E\{m(H, t+1)\} \geq m(H, t) \frac{\bar{f}(H, t)}{\bar{f}(\mathbf{A}(t))} \left[1 - p_c \cdot \frac{\delta(H)}{\ell - 1} - o(H)p_m \right], \quad (2)$$

where $m(H, t)$ is the number of representatives of H in the population at time t (Grefenstette & Baker, 1989), $\bar{f}(H, t)$ is the average fitness of the representatives of H in the present population, $\bar{f}(\mathbf{A}(t))$ is the average fitness of the present population, p_c is the crossover probability, and p_m is the mutation probability. Based on (2), it has been concluded that small, low-order schemata with above-average performance are allocated exponentially increasing

trials in subsequent generations (Goldberg, 1989a). An important observation in the schema theory is that each binary string *implicitly* searches or samples 2^l schemata. According to the theory, this implicitly acquired information is then used for trial allocation to schemata and to generate increasingly better strings. It has been argued that implicit parallelism leverages the power of genetic algorithms (Goldberg, 1989a), and allows them to avoid the obstacles of high dimensionality (Holland, 1975). Equation (2) is often referred to as the *Schema Theorem* or the *Fundamental Theorem of Genetic Algorithms* (Goldberg, 1989a).

The schema theory will now be evaluated according to the suitability criteria established at the beginning of this section.

1. The allocation of trials to schemata in a manner consistent with the schema theorem is certainly well grounded to the procedural elements. However, schema information is not used in the procedure for trial allocation or any other purpose. Therefore, the use of acquired schema information to guide or affect genetic algorithm behavior has no tangible basis and is not well grounded (Peck, 1993, §3.2.5).
2. The schema theory has lead to useful, verifiable predictions (*e.g.*, see (Fitzpatrick & Grefenstette, 1988; Goldberg, Deb & Clark, 1992; Goldberg, Deb & Clark, 1993)). However, the schema theory is inexact due to the inequality in (2). Furthermore, the schema theory and the building block hypothesis are unable to explain how genetic algorithms systematically generate improved candidate solutions, since they depend on the use of implicitly acquired schema information (Peck, 1993, §3.2.5).
3. The schema theory, as presented in this paper, is not robust with respect to algorithmic variations (Peck, 1993, §3.2.5). Genetic algorithm variants using fitness scaling, ranking, and/or real (floating point) encodings are difficult, if not impossible, to explain within the context of the schema theory. The attempts that have been made require a new interpretation of the schema theory or higher-order abstractions (Whitley, 1989; Goldberg, 1991a; Goldberg, 1991b). Similar algorithms, such as *evolution strategies*

and *evolutionary programming* (Bäck & Schwefel, 1993), are beyond the scope of the schema theory.

It has also been observed that schema-based analysis of genetic algorithm behavior is greatly complicated by the difficulties in associating properties to schemata (Forrest & Mitchell, 1993; Grefenstette & Baker, 1989; Grefenstette, 1991; Grefenstette, 1993; Peck, 1993; Peck & Dhawan, 1993). Finally, since genetic algorithms do not use schema information, there is no basis to conclude that genetic algorithms realize advantages from implicit parallelism (Peck, 1993).

2.2 Alternative Analyses of Genetic Algorithms

While the primary basis of genetic algorithm analysis has been the schema theory, other types of analysis have been pursued as well. The primary bases of alternative analysis have been Markov chain and simulated annealing theory. Most of the analyses in the literature have only sought to address specific issues, have made simplifying assumptions, or have not been dependent on the distinguishing characteristics of genetic algorithms (De Jong, 1975; Goldberg & Segrest, 1987; Rabinovich & Wigderson, 1991; Eiben, Aarts & Hee, 1991; Davis & Principe, 1991).

The theory presented in (Vose & Liepins, 1991a; Nix & Vose, 1992; Vose, 1993a) represents the most accurate and complete alternative theory of genetic algorithm behavior in the literature. In (Vose & Liepins, 1991a), Vose and Liepins present a novel, algebraic formalization and analysis of a simple genetic algorithm. Using Markov chain analysis, with the state defined by the composition of an infinite sized population, the trajectory of the expected populations is modeled, and the conditions for convergence to the absorbing states of the transition mapping are derived. In (Nix & Vose, 1992), the formalism of the Vose and Liepins model is applied to a simple genetic algorithm with a finite population size. It is concluded that, as the population size increases, the asymptotic behavior of the steady state distributions may be characterized in terms of the Vose and Liepins model. In (Vose, 1993a),

the two preceding works are further tied together, and the *GA-surface* is introduced. The GA-surface, which is composed of the points corresponding to populations, may be used to provide a geometric interpretation of genetic search and to explain population trajectories.

The theory contained in (Vose & Liepins, 1991a; Nix & Vose, 1992; Vose, 1993a) will now be interpreted in the context of the criteria established at the beginning of this section:

1. The construction and operation of the population transition operators is well grounded in the procedural elements and generating mechanisms of genetic algorithms. In fact, the representations in (Nix & Vose, 1992) and (Vose & Liepins, 1991a) are exact for finite and infinite populations, respectively.
2. Since the representations are exact, any phenomena observed of genetic algorithms will be explainable within their contexts. As an example, observations of punctuated equilibrium are explainable in the context of the infinite population representation. Furthermore, many predictions regarding short and long term behavior have been derived from this analysis.
3. Markov chain representations may be generated for nearly any algorithmic variant. Derived properties must naturally be proved for each variant.

The above analysis suggests that a suitable theory for genetic algorithm analysis has been constructed. There is, however, a subtle caveat to this conclusion: the explanatory power of this work is hampered by lumping genetic algorithm behavior into a population transition operator. There are many low-level phenomena of genetic algorithms that are not adequately understood, and a high-level, unitary abstraction such as a population transition operator may have difficulty explaining them. A level of abstraction operating between the low-level abstraction of the procedure and the high-level abstraction of the transition operator is desired.

3 Global Random Search Methods: An Overview

This section reviews the theory of global random search methods. This theory serves as the basis for an alternative theory of genetic algorithm behavior, which is presented in Section 4. The presentation throughout this section primarily summarizes and clarifies the analysis and results presented by Zhigljavsky (Zhigljavsky, 1991). A more thorough summary of these results is presented in (Peck, 1993).

This section begins with an introduction to global search methods. This is followed by a presentation of basic global random search methods. Finally, generational methods and their convergence properties are examined.

3.1 Introduction and Notation

In the typical global optimization problem, it is desired to optimize an objective function, which may be a mathematical expression or the output of an algorithm, process, experiment, or system. Let \mathcal{X} denote a set referred to as the feasible region and $f : \mathcal{X} \rightarrow \mathbb{R}^1$ be the objective function. In the global minimization problem, it is desired to approximate either the value

$$f^* = \inf_{x \in \mathcal{X}} f(x), \quad (3)$$

the point $x^* \in \mathcal{X}$ at which the minimal value f^* is attained,

$$x^* = \arg \min_{x \in \mathcal{X}} f(x), \quad (4)$$

or both. The global minimizer, x^* , is not generally unique.

Approximating f^* and a point $x^* = \arg \min f$ is usually interpreted as finding a point in either the set

$$A(\delta) = \{x \in \mathcal{X} : |f(x) - f(x^*)| \leq \delta\}, \quad (5)$$

or the set

$$B(\varepsilon) = B(x^*, \varepsilon, \rho) = \{x \in \mathcal{X} : \rho(x, x^*) \leq \varepsilon\}, \quad (6)$$

where ρ is the given metric on \mathcal{X} , δ , and ε determine the accuracy of the approximation with respect to the function and argument values (Zhigljavsky, 1991, pg. 2).

In the global maximization problem, alternatively, the objective is to approximate either the value

$$M = \sup_{x \in \mathcal{X}} f(x), \quad (7)$$

the global maximizer, which will also be denoted x^* , where

$$x^* = \arg \max_{x \in \mathcal{X}} f(x), \quad (8)$$

or both. The meaning of x^* will be understood through context. It should also be noted that by substituting $-f$ for f , the maximization problem may be converted into a minimization problem, and vice versa. To avoid redundancy, only the minimization problem will be addressed for the remainder of this and the next subsection.

Generally, a global minimization method is a procedure for constructing a sequence $\{x_k\}$ of points in \mathcal{X} that converges to a point at which the global minimizer, f^* , is attained or approximated (Zhigljavsky, 1991, pg. 1). The nature of convergence depends on the optimization method. For example, convergence may be of the values of $f(x_k)$ to f^* or of the sequence $\{x_k\}$ to a probability measure concentrated at x^* . This procedure may use *a priori* information about \mathcal{X} or f , such as values of f , its derivatives, or the presence and nature of random noise.

The complexity of the optimization problem is dependent on the properties of \mathcal{X} and f . Furthermore, there exists a duality between the corresponding properties (Zhigljavsky, 1991, pg. 2). Specifically, if \mathcal{X} is complex but f is simple, then the optimization problem may be reformulated such that \mathcal{X} is simple and f is complex, and vice versa.

As stated above, the nature of \mathcal{X} effects the complexity of the optimization problem and should be considered in the selection of the optimization technique. In general, unlike local optimization, global optimization cannot be done if \mathcal{X} is not bounded. Some techniques require that \mathcal{X} possess certain properties (*e.g.*, that \mathcal{X} be closed, compact, connected, etc.).

Other important considerations include the choice of a metric on \mathcal{X} , techniques for reducing the complexities associated with problem constraints, and the dimension n of \mathcal{X} when $\mathcal{X} \subset \mathbb{R}^n$ (Zhigljavsky, 1991, pg. 3)

The optimization method is typically selected, in part, based on the functional class, \mathcal{F} , of f , which is determined by prior knowledge of f . The chosen functional class corresponds to a model of f . The wider the functional class \mathcal{F} is, the wider the class of allowable problems is, and the less efficient the algorithms are (Zhigljavsky, 1991, pg. 3).

3.2 Basic Global Random Search Methods

Global random search methods may be classified as passive or adaptive. Passive methods, such as uniform random sampling (pure random search), proceed without exploiting information learned about f on \mathcal{X} . Consequently, these methods are typically quite simple, but they are also quite inefficient. Adaptive methods, conversely, use acquired and *a priori* information to improve their efficiency. For a brief survey of adaptive methods, see (Zhigljavsky, 1991, pg. 82).

3.2.1 Formalization of Global Random Search Methods

The following procedure represents a generalization and formalization of global random search methods. It is intended to serve as the basis of comparison and discussion of the various methods considered in this paper.

Procedure 2 Formal Scheme of Global Random Search (Zhigljavsky, 1991, Algorithm 3.1.5, pg. 85)

1. Set $k = 1$, choose a probability distribution P_1 on \mathcal{X} .
2. Sample N_k times the distribution P_k to obtain the points

$$x_1^{(k)}, \dots, x_{N_k}^{(k)}.$$

At each of these points, evaluate f , possibly with random noise.

3. Using a fixed, algorithm-dependent rule, construct the probability distribution P_{k+1} on \mathcal{X} .
4. If the stopping criterion is satisfied, then stop; otherwise, set $k = k + 1$ and continue with Step 2.

This procedure illustrates that any global random search method is iterative. Furthermore, at each iteration a suitably constructed distribution is sampled (Zhigljavsky, 1991, pg. 85). In Markovian methods, $N_k = 1$ for all k .

The distributions $\{P_{k+1}\}$ determine how *a priori* information and the information acquired during the search process is derived and exploited by the search algorithm. Without loss of generality, the distributions may be written in the form

$$P_{k+1}(dx) = \int_{\mathcal{X}} R_k(dz) Q_k(z, dx), \quad (9)$$

where R_k is a probability distribution on \mathcal{X} and $Q_k(z, \cdot)$ is a Markovian transition probability (Zhigljavsky, 1991, pg. 85). The transition probability, $Q_k(z, \cdot)$, is a measurable, nonnegative function with respect to the first argument and a probability measure with respect to the second. Sampling this distribution is performed by sampling $R_k(dz)$ to obtain z , then sampling $Q_k(z, dx)$ to obtain x , the desired sample. As shown below, R_k and $Q_k(z, \cdot)$, serve two distinct roles in the search strategy.

The distribution R_k comprises the global aspects of the search strategy. Accordingly, R_k is constructed using globally derived information about f , and a point from all of \mathcal{X} is chosen when sampling R_k . The method for constructing R_k largely determines the general structure of the algorithm, and it is the typical basis for algorithm classification. Common classes of algorithms include Markovian, generational, and branch and bound.

The distribution $Q_k(z, \cdot)$ comprises the local aspects of the search strategy. When sampling $Q_k(z, \cdot)$, a point in the neighborhood of z is selected. The term *neighborhood* should be interpreted to mean “with large probability near enough (Zhigljavsky, 1991, pg. 86).” The

nature of $Q_k(z, \cdot)$ largely determines the tradeoff between the accuracy of the final result and the efficiency of the search. A simple choice of $Q_k(z, \cdot)$ is

$$Q_k(z, dx) = \frac{\varphi_k(x - z)dx}{\int_{\mathcal{X}} \varphi_k(y - z)dy}, \quad (10)$$

where φ_k is a chosen distribution density in \mathbb{R}^n . The denominator of (10) is a normalization constant. A random realization x_k in \mathcal{X} from the distribution in (10) may be obtained by repeatedly sampling φ_k to obtain a realization ξ_k until $z + \xi_k \in \mathcal{X}$, then setting $x_k = z + \xi_k$. The distribution described above is the method of choice when random noise is present in the evaluations of f (Zhigljavsky, 1991, pg. 86). It is also useful as a component of other distributions.

When f is evaluated without noise, the following distributions for $Q_k(z, \cdot)$ are often preferred:

$$Q_k(z, A) = \int_{\mathcal{X}} 1_{[x \in A, f(x) \leq f(z)]} T_k(z, dx) + 1_A(z) \int_{\mathcal{X}} 1_{[f(z) < f(x)]} T_k(z, dx), \quad (11)$$

where $T_k(z, dx)$ is a Markovian transition probability of the form expressed in (10) and 1_A is the indicator of set A :

$$1_A(x) = 1_{[x \in A]} = \begin{cases} 1 & \text{if } x \in A \\ 0 & \text{if } x \notin A. \end{cases} \quad (12)$$

The first integral represents the probability of sampling a point $x \in A$ for which $f(x) \leq f(z)$. The second integral, which only contributes to the sum if $z \in A$, is the probability of sampling a point $x \in \mathcal{X}$ for which $f(x) > f(z)$. A realization x_k from (11) may be obtained by sampling the distribution $T_k(z, \cdot)$ to get ξ_k and setting

$$x_k = \begin{cases} \xi_k & \text{if } f(\xi_k) \leq f(z) \\ z & \text{otherwise.} \end{cases}$$

Other methods for constructing $Q_k(z, \cdot)$ exist. In fact, it is not necessary to know the analytical form of $Q_k(z, \cdot)$, it is only necessary that a method for sampling, such as an algorithm, exists (Zhigljavsky, 1991, pg. 87). Furthermore, $Q_k(z, \cdot)$ may be constructed using *a priori* information or information acquired during the search.

3.2.2 General Convergence Results

In this section, Zhigljavsky's general results on the convergence of global random search methods will be presented without proof. For the proofs, the interested reader should refer to (Zhigljavsky, 1991, §3.2). Without loss of generality, it will be assumed that $N_k = 1$ for all $k = 1, 2, \dots$ such that a separate distribution P_k is constructed for each sampled point, $x_k = x_1^{(k)}$.

Theorem 1 *Let f be continuous in the vicinity of a global minimizer x^* of f , and assume that*

$$\sum_{k=1}^{\infty} q_k = \infty \quad (13)$$

for any $x \in \mathcal{X}$ and $\varepsilon > 0$ where

$$q_k = q_k(x^*, \varepsilon) = \text{vrai inf}_{\Xi_{k-1}} P_k(B(\varepsilon)), \quad \Xi_{k-1} = \{x_1, \dots, x_{k-1}\},$$

and $\text{vrai inf } \eta$ is the essential infimum of a random variable η :

$$\text{vrai inf } \eta = \sup \{a : \Pr\{\eta \geq a\} = 1\}.$$

Then for any $\delta > 0$ the sequence of random vectors x_k generated by Procedure 2 with $N_k = 1$ for $k = 1, 2, \dots$ falls infinitely often into the set $A(\delta)$ with probability one.

Theorem 1 makes use of the probabilities, for each iteration, of falling into an arbitrarily small set around a global optimizer. It shows that if the sum of these probabilities is unbounded, then infinitely many evaluations of f will be arbitrarily close to the global optimum. This theorem applies even when f is evaluated with random noise. Since the location of any global optimizer is typically not known *a priori*, it is sufficient instead to require that Theorem 1 apply to every $x \in \mathcal{X}$, in addition to sets around global optimizers. This stricter, yet simpler, requirement may be expressed:

$$\sum_{k=1}^{\infty} \text{vrai inf}_{\Xi_{k-1}} P_k(B(x, \varepsilon)) = \infty, \quad (14)$$

for all $\varepsilon > 0$, $x \in \mathcal{X}$.

There are many ways of selecting probability distributions P_k such that (14) is satisfied. A common approach is to select the probability distributions P_k according to

$$P_k = \alpha_k P_{\mathcal{X}} + (1 - \alpha_k) G_k, \quad (15)$$

where $0 \leq \alpha \leq 1$, $P_{\mathcal{X}}$ is the uniform distribution on \mathcal{X} , and G_k is an arbitrary distribution on \mathcal{X} . A realization, x_k , from (15) may be obtained by sampling $P_{\mathcal{X}}$ with probability α_k and G_k with probability $1 - \alpha_k$. To satisfy (14), it is sufficient to require

$$\sum_{k=1}^{\infty} \alpha_k = \infty.$$

3.3 Methods of Generations

Generational methods, also called *methods of generations* in the literature, sequentially sample probability distributions that are asymptotically concentrated in the vicinity of a global optimizer multiple times. Each of these multiple samplings is referred to as a generation. These methods, which were first proposed in the late 1960's, are based upon the three following heuristics (Zhigljavsky, 1991, pg. 186):

- i. New samples of f should most often be obtained in the vicinity of previous, high-performance samples,
- ii. The number of new samples in the vicinity of a previous sample must depend on the observed value of f at that sample,
- iii. The breadth of the sampling distribution around the previous samplings should decrease as the global optimizer is approached.

Generational methods have many desirable properties. In exchange for their inefficiency at solving *easy* global optimization problems, they are suitable for a wide range of problem domains. In particular, they may be applied to very complex problems and they are

applicable when noise is present. Finally, as shown in Subsection 3.3.2, they have provable convergence properties.

In this section, it will be assumed that the feasible region, \mathcal{X} is a compact metric space of an arbitrary type. Furthermore, it will be assumed that the maximization problem is being considered.

3.3.1 Presentation of Generational Methods

The following procedure satisfies the three heuristics. It is based on the supposition that the result of evaluating f at a sample point $x \in \mathcal{X}$ and iteration k is a nonnegative random variable $y_k(x) = f(x) + \xi_k(x)$, where $\xi_k(x)$ is also a random variable. \mathcal{B} is the σ -algebra of the Borel subsets of \mathcal{X} .

Procedure 3 Generalized Method of Generations Algorithm with Randomization

1. Choose a distribution P_1 on $(\mathcal{X}, \mathcal{B})$ and set $k = 1$.
2. Sample N_k times the distribution P_k to obtain the points $x_1^{(1)}, \dots, x_{N_k}^{(1)}$.
3. Evaluate the random variables $y_k(x_j^{(k)})$ at the points $x_j^{(k)}$, where $y_k(x) = f_k(x) + \xi(x) \geq 0$ with probability one, and f_k is an auxiliary nonnegative function constructed using the observed values of f at the points $x_j^{(i)}$ for $j = 1, \dots, N_i, i = 1, \dots, k$. If

$$\sum_{j=1}^{N_k} y_k(x_j^{(k)}) = 0,$$

then repeat the sampling by returning to Step 2.

4. Construct the next distribution according to

$$P_{k+1}(dx) = \sum_{j=1}^{N_k} p_j^{(k)} Q_k(x_j^{(k)}, dx) \quad (16)$$

where

$$p_k^{(k)} = \frac{y_k(x_k^{(k)})}{\sum_{i=1}^{N_k} y_k(x_i^{(k)})}. \quad (17)$$

5. If the stopping criterion is satisfied, then stop; otherwise, substitute $k + 1$ for k and go to Step 2.

The distribution P_{k+1} in (16) is sampled using superposition: first the discrete distribution

$$\varepsilon_k = \left\{ \begin{array}{c} x_1^{(k)}, \dots, x_{N_k}^{(k)} \\ p_1^{(k)}, \dots, p_{N_k}^{(k)} \end{array} \right\} \quad (18)$$

is sampled, then the distribution $Q_k(x_j^{(k)}, \cdot)$ is sampled for each realization $x_j^{(k)}$ (Zhigljavsky, 1991, pg. 188). It will be assumed in the theoretical analysis of Procedure 3 that (16) will be sampled in this manner. In practice, however, variance reduction techniques are typically applied to the sampling procedure (Zhigljavsky, 1991, pp. 188–189). These techniques ensure that some of the *best* points are sampled with probability one.

In Procedure 3, auxiliary, nonnegative functions, f_k , are used to construct P_{k+1} . These functions should reflect the properties of f . For example, f_k should, on the average, be greater where f is great and smaller where f is small. The choice of f_k can greatly affect the quality of the resulting algorithm. Zhigljavsky suggests that the construction of these functions should be done with a technique for extracting and using information about the objective function during the search or be based upon some technique of objective function estimation (Zhigljavsky, 1991, pg. 189).

Procedure 3 may be terminated when a prescribed number of iterations have been executed or according to some other criterion. Zhigljavsky suggests termination when the desired accuracy has been obtained. This may be determined using the methods for estimating M described in (Zhigljavsky, 1991, Ch. 4).

There are also sequential variants of Procedure 3 (Zhigljavsky, 1991, §5.4). The distinguishing characteristics of these algorithms are that the sampling distributions $P_{k+1}(dx)$ may be constructed using points from all previous iterations, and, except for the first iteration, only one sample is obtained per iteration.

3.3.2 Convergence Properties

In this subsection, the convergence properties of the global random search methods described by Procedure 3 will be considered. To prove that the sampling distributions of methods of generations weakly converge to the probability measure concentrated at a global optimum, Zhigljavsky places key requirements upon the local sampling components, Q_k , and the global sampling components, R_k . Of these requirements, two are placed on the local sampling components:

1. The breadth of the distributions Q_k must be reduced as the algorithm proceeds such that the sequence weakly converges to a probability measure concentrated at the point where it is located.
2. The distributions Q_k must somehow be constrained so that their expansive nature cannot overcome the convergence caused by the global sampling components, R_k . *A fortiori*, these distributions must be designed to prevent diffusion away from global optima in the absence of selective convergence; otherwise, additional assumptions about the objective function, f , would be required.

Without the first requirement it would not be possible to prove convergence of the sampling distributions to a probability measure concentrated at a global optimum or any other point. Zhigljavsky satisfies the second requirement in two ways. In Corollary 3 below, a form of local elitism is used to prevent dispersion of the sampling distribution away from global optima. In Corollary 4 below, the search breadth of the distributions Q_k is required to be finite, and the breadth of these distributions are required to decrease rapidly enough so that the search range becomes bounded. Finally, the distributions R_k are required to be in the form of proportional selection, (17) or (1). Heuristically, the sampling distributions of methods of generations converge to the global sampling distributions

$$\frac{f^k(x)\mu(dx)}{\int f^k(z)\mu(dz)}$$

due to the requirements placed on the local sampling distributions Q_k . Furthermore, as shown in Lemma 2, these distributions converge to global optima.

Auxiliary Statements Below, two auxiliary lemmas of considerable importance and two associated corollaries are presented. Appendix B presents the assumptions upon which these results are based. The proofs for these results are presented in (Zhigljavsky, 1991, §5.2.2).

Lemma 1 *If the assumptions (a), (b), (c), (e), (f), (g), and (s) are satisfied, then*

1. *the random variables with the distribution $P_M(dx_1, \dots, dx_M)$ are symmetrically dependent;*
2. *the marginal distributions $\tilde{P}_M(dx) = P_M(dx, \mathcal{X}, \dots, \mathcal{X})$ are representable as*

$$\tilde{P}_M(dx) = \frac{\int \tilde{R}_N(dz) f(z) Q(z, dx)}{\int \tilde{R}_N(dz) f(z)} + \Delta_N(dx), \quad (19)$$

where $\tilde{R}_N(dz) = R_N(dz, \mathcal{X}, \dots, \mathcal{X})$; and

3. *the signed measures Δ_N converge to zero in variation for $N \rightarrow \infty$ with the rate $N^{-1/2}$, i.e., $\text{var}(\Delta_N) = O(N^{-1/2})$, $N \rightarrow \infty$.*

By substituting f_k , N_k , N_{k+1} , $P(k, N_{k-1}; \cdot)$, $P(k+1, N_k; \cdot)$, $P(k+1, N_k; dx) = P(k+1, N_k; dx, \mathcal{X}, \dots, \mathcal{X})$, and $\Delta(k, N_k, \cdot)$ for f , N , M , $R_N(\cdot)$, $P_M(\cdot)$, $\tilde{P}_M(dx)$, and $\Delta_N(\cdot)$, respectively, and applying Lemma 1, Zhigljavsky obtains the following assertion.

Corollary 1 *Let (a), (b), (c), and (e) be met. Then for any $k = 1, 2, \dots$ and $N_k = 1, 2, \dots$ the following equality holds for the unconditional distribution of random elements $x_j^{(k)}$:*

$$P(k+1, N_k; dx) = \frac{\int P(k, N_{k-1}; dz) f_k(z) R(k, N_k, z; dx)}{\int P(k, N_{k-1}; dz) f_k(z)} \quad (20)$$

where

$$R(k, N_k, z; dx) = Q_k(z, dx) + \Delta(k, N_k; dx),$$

and the signed measures $\Delta(k, N_k; \cdot)$ converge in variation to zero for $N \rightarrow \infty$ with the rate of order $N_k^{-1/2}$ for any $k = 1, 2, \dots$

This leads to the next corollary.

Corollary 2 *Let (a), (b), (c), and (e) be satisfied. Then for any $k = 1, 2, \dots$ the sequence of distributions $P(k+1, N_k; \cdot)$ converges in variation for $N_k \rightarrow \infty$ to the limit distributions $P_k(\cdot)$ and*

$$P_{k+1}(dx) = \frac{\int P_k(dz) f_k(z) Q_k(z, dx)}{\int P_k(dz) f_k(z)} \quad (21)$$

Loosely speaking, Lemma 1 and Corollaries 1 and 2 above concern the distributions constructed by generational methods. The following lemma concerns the distributions constructed by (17) alone. Appendix A provides a definition and three alternative characterizations of weak convergence.

Lemma 2 *Let (c), (d), (h), (i), and (j) be satisfied. Then the sequence of distributions*

$$P_{k+1}(dx) = \frac{f^m(x) \mu(dx)}{\int f^m(z) \mu(dz)} \quad (22)$$

weakly converges to $\varepsilon^(dx) = \varepsilon_{x^*}(dx)$ for $m \rightarrow \infty$.*

Convergence Properties The sufficient conditions for the weak convergence of the distribution sequences (20) and (21) to $\varepsilon^*(dx)$ for $k \rightarrow \infty$ will now be presented. The proofs for these results are presented in (Zhigljavsky, 1991, 5.2.3).

Theorem 2 *Let the conditions (c), (d), (e), (h), (i), and (j) be satisfied as well as (k) and (m) or (l) and (n). Then the distribution sequence determined through (21) or, respectively, through (20) weakly converges to $\varepsilon^*(dx)$ for $k \rightarrow \infty$.*

With the exception of conditions (m) and (n), all of the required conditions for Theorem 2 are natural and reasonable. As mentioned previously, it is of great interest to determine

the sufficient conditions for the satisfaction of (m) and (n). In (Zhigljavsky, 1991, §5.2.3), Zhigljavsky formulates the sufficient conditions for distribution convergence to $\varepsilon^*(dx)$ for the two theoretically most important ways of choosing the transition probabilities $Q_k(z, dx)$, as follows.

Corollary 3 *Let the conditions (c), (d), (e), (h), (i), (j), (o), (p), (q), and (t) be satisfied. Furthermore, let (k) be satisfied for the transition probabilities $T_k(x, dz)$ of (59). Then the sequence of distributions determined by (21) weakly converges to $\varepsilon^*(dx)$ for $k \rightarrow \infty$.*

Corollary 4 *Let the conditions (e), (h), (i), (j), (q), (r), and (t) be satisfied. Then the sequence of distributions determined by (21) weakly converges to $\varepsilon^*(dx)$ for $k \rightarrow \infty$.*

Zhigljavsky asserts that, like Theorem 2, Corollaries 3 and 4 may be reformulated to demonstrate the convergence of (20) to $\varepsilon^*(dx)$. Corollary 4, the more non-trivial of the two, was then reformulated and proved.

Corollary 5 *Let the conditions formulated in Corollaries 1 and 4 be satisfied. Then there exists a sequence of natural numbers N_k ($N_k \rightarrow \infty$ for $k \rightarrow \infty$) such that the sequence of distributions $P(k + 1, N_k; dx)$ determined by (20) weakly converges to $\varepsilon^*(dx)$ for $k \rightarrow \infty$.*

4 Genetic Algorithms as Global Random Search Methods

Genetic algorithms are global random search methods. Accordingly, it is argued that genetic algorithm behavior is best described by the construction and evolution of the sampling distributions. Furthermore, it is preferred that these sampling distributions be described relative to the phenospace, rather than the genospace. However, genotypic sampling distributions are equally useful when the distribution of candidate solutions across the genospace is understood or known. Matching the simplicity of the genetic algorithm itself, this perspective and the theory associated with it is remarkably simple. Furthermore, it will be shown that

this is a suitable theory for genetic algorithm behavior according to the criteria established in Section 2.

The genotypic sampling distributions of genetic algorithms have been described previously in the literature. The sampling distributions arising from proportional selection and mutation are presented in (Davis & Principe, 1991). Those resulting from proportional selection and one-point crossover are described in (Bridges & Goldberg, 1987; Whitley, 1993). Statistical measures derived from recombination operators and their relationship to the objective function are presented in (Manderick, de Weger & Spiessens, 1991). The sampling distributions constructed using proportional selection, one-point crossover, and mutation are presented in (Vose & Liepins, 1991a). Recently, Vose independently recognized that the interpretation of the population transition operators as sampling distributions is a unifying theme that nicely connects his finite and infinite population models of genetic algorithms (Vose, 1993b).

This section applies the formalism and insights of the theory of global random search methods in Section 3 to genetic algorithms. First, the genetic algorithm is reformulated and generalized in terms of phenotypic search. Genetic algorithm behavior is then described in terms of three heuristics related to the procedural elements of genetic algorithms. Finally, the suitability of sampling distribution theory for describing genetic algorithm behavior is considered in the context of the criteria established in Section 2.

4.1 Reformulating the Genetic Algorithm

The canonical genetic algorithm searches the discrete space of attainable strings \mathcal{A} , where a single string is denoted A or A_i . In Procedure 4, the canonical genetic algorithm is expressed in the form of the *methods of generations* in Subsection 3.3.1. It is assumed that if the objective function, $\tilde{f} : \mathcal{A} \rightarrow \mathbb{R}^1$, is evaluated with noise at iteration k , then the result is a nonnegative random variable $\tilde{y}_k(A) = \tilde{f}(A) + \xi_k(A)$, where $\xi_k(A)$ is a random variable.

Procedure 4 The canonical genetic algorithm as a generational global random search method.

1. Choose a distribution P_1 on \mathcal{A} and set $k = 1$.
2. Sample N_k times P_k to obtain the strings $A_1^{(k)}, \dots, A_{N_k}^{(k)}$.
3. Evaluate the random variables $\tilde{y}_k(A_j^{(k)})$ at the strings $A_j^{(k)}$, where $\tilde{y}_k(A) = \tilde{f}_k(A) + \xi_k(A) \geq 0$ with probability one, \tilde{f}_k is an auxiliary nonnegative function constructed using the observed values of \tilde{f} at the strings $A_j^{(i)}$ for $j = 1, \dots, N_i, i = 1, \dots, k$, and $\tilde{f} : \mathcal{A} \rightarrow \mathbb{R}^1$ is the fitness or objective function. If

$$\sum_{j=1}^{N_k} \tilde{y}_k(A_j^{(k)}) = 0,$$

repeat the sampling by returning to Step 2.

4. Construct the next distribution according to

$$P_{k+1}(A_i) = \sum_{j'=1}^{N_k} \sum_{j''=1}^{N_k} p_{j'}^{(k)} p_{j''}^{(k)} \tilde{Q}_k(A_{j'}, A_{j''}, A_i), \quad (23)$$

where

$$p_j^{(k)} = \frac{\tilde{y}_k(A_j^{(K)})}{\sum_{i=1}^{N_k} \tilde{y}_k(A_i^{(k)})}. \quad (24)$$

5. If the stopping criterion is satisfied, then stop; otherwise, substitute $k + 1$ for k and go to Step 2.

The construction of the sampling distributions $\{P_{k+1}\}$ in (23) is consistent with Lemma 1 in (Vose & Liepins, 1991a) and it proceeds in two stages: a global phase and a local phase. The realizations $A_{j'}$ and $A_{j''}$ are obtained using global information about \tilde{f} contained in the population and (24). The local phase corresponds to recombination, which encompasses both crossover and mutation, and is performed with the transition probability $\tilde{Q}_k(A_{j'}, A_{j''}, \cdot)$. The emphasis on the use of two samples for the construction of the transition probability distribution is the distinguishing characteristic of genetic algorithms from other global random search methods, including evolutionary programming (Fogel & Atmar, 1990; Bäck &

Schwefel, 1993) and evolutionary strategies (Bäck & Schwefel, 1993; Bäck, Hoffmeister & Schwefel, 1991). It is on the basis of these two samples and a similarity measure that the locality of $\tilde{Q}_k(A_{j'}, A_{j''}, \cdot)$ is typically determined. This is discussed further in Subsection 4.2.

The distribution P_{k+1} in (23) is sampled using superposition: first the discrete distribution

$$\varepsilon_k = \left\{ \begin{array}{c} A_1^{(k)}, \dots, A_{N_k}^{(k)} \\ p_1^{(k)}, \dots, p_{N_k}^{(k)} \end{array} \right\} \quad (25)$$

is sampled twice, then the distribution $\tilde{Q}_k(A_{j'}^{(k)}, A_{j''}^{(k)}, \cdot)$ is sampled for each pair of realizations $A_{j'}^{(k)}$ and $A_{j''}^{(k)}$. The transition probability $\tilde{Q}_k(A_{j'}^{(k)}, A_{j''}^{(k)}, A)$ describes the probability of obtaining the realization A given the pair $A_{j'}^{(k)}$ and $A_{j''}^{(k)}$. The distribution P_{k+1} in (23) may also be sampled using a variance reduction technique (for examples, see (Baker, 1987; Baker, 1989; Zhigljavsky, 1991)). Finally, the distributions $\{P_{k+1}\}$ in (23) may alternatively be constructed to generate a pair of samples (Peck, 1993),

$$P_{k+1}(A_{i'}, A_{i''}) = \sum_{j'=1}^{N_k} \sum_{j''=1}^{N_k} p_{j'}^{(k)} p_{j''}^{(k)} \tilde{Q}_k(A_{j'}^{(k)}, A_{j''}^{(k)}, A_{i'}, A_{i''}), \quad (26)$$

where the transition probability $\tilde{Q}_k(A_{j'}^{(k)}, A_{j''}^{(k)}, A_{i'}, A_{i''})$ describes the probability of realizing the pair $(A_{i'}, A_{i''})$ given the pair $(A_{j'}^{(k)}, A_{j''}^{(k)})$.

The auxiliary functions \tilde{f}_k in Step 3 should reflect the properties of \tilde{f} . That is, they should be greater when \tilde{f} is greater and smaller when \tilde{f} is smaller. Common choices of \tilde{f}_k include functions for fitness scaling and ranking. These functions may, in general, be constructed using any subset of the previous samples. Generational genetic algorithms, however, typically only use $A_1^{(k-1)}, \dots, A_{N_{k-1}}^{(k-1)}$.

The genetic algorithm may also be described in terms of the phenospace or feasible space \mathcal{X} . In genetic algorithms, each string or element A of \mathcal{A} is an encoding of a candidate solution x , which is an element of the feasible space \mathcal{X} . Due to the mapping $\mathcal{M} : \mathcal{A} \rightarrow \mathcal{X}$, the sampling distribution $\tilde{Q}_k(A_{j'}, A_{j''}, \cdot)$ on \mathcal{A} constructed by selection and recombination also imposes a sampling distribution $Q_k(z', z'', \cdot)$ on \mathcal{X} . In other words, the realization x obtained from $Q_k(\mathcal{M}(A_{j'}), \mathcal{M}(A_{j''}), \cdot)$ is identical to $\mathcal{M}(A_i)$, where A_i is the realization

obtained from $\tilde{Q}_k(A_{j'}, A_{j''), \cdot)$. The genetic algorithm can then be generalized to search the phenospace, where the sampling distributions $\{P_{k+1}\}$ are constructed with respect to \mathcal{X} according to

$$P_{k+1}(dx) = \int_{\mathcal{X}} \int_{\mathcal{X}} R_k(dz') R_k(dz'') Q_k(z', z'', dx), \quad (27)$$

where R_k is a probability measure on \mathcal{X} and $Q_k(z', z'', \cdot)$ is a transition probability such that it is a measurable function with respect to the first two arguments and a probability measure with respect to the third. The distributions $\{P_{k+1}\}$ are typically sampled using superposition: first realizations z' and z'' are obtained by sampling R_k , then $Q_k(z', z'', \cdot)$ is sampled to obtain x . Finally, the distributions $\{P_{k+1}\}$ in (27) may alternatively be constructed to generate a pair of samples (Peck, 1993).

In analogy to (26), the distributions $\{P_{k+1}\}$ may alternatively be constructed according to

$$P_{k+1}(dx', dx'') = \int_{\mathcal{X}} \int_{\mathcal{X}} R_k(dz') R_k(dz'') Q_k(z', z'', dx', dx''), \quad (28)$$

where, once again, R_k is a probability measure on \mathcal{X} and $Q_k(z', z'', dx', dx'')$ is a transition probability such that it is a measurable function with respect to the first two arguments and a probability measure with respect to the last two arguments. For the purposes of analysis and discussion only (27) will be considered further.

To generate distributions consistent with (27), the genetic algorithm may be generalized in the following form, where \mathcal{B} is the σ -algebra of the Borel subsets of \mathcal{X} :

Procedure 5 The generalized genetic algorithm as a generational global random search method.

1. Choose a distribution P_1 on $(\mathcal{X}, \mathcal{B})$ and set $k = 1$.
2. Sample N_k times P_k to obtain the points $x_1^{(k)}, \dots, x_{N_k}^{(k)}$.
3. Evaluate the random variables $y_k(x_j^{(k)})$ at the points $x_j^{(k)}$, where $y_k(x_j^{(k)}) = f_k(x_j^{(k)}) + \xi_k(x_j^{(k)}) \geq 0$ with probability one, f_k is an auxiliary nonnegative function constructed

using the observed values of f at the points $x_j^{(i)}$ for $j = 1, \dots, N_i, i = 1, \dots, k$, and $f : \mathcal{X} \rightarrow \mathbb{R}^1$ is the fitness or objective function. If

$$\sum_{j=1}^{N_k} y_k(x_j^{(k)}) = 0,$$

repeat the sampling by returning to Step 2.

4. Construct the next distribution according to

$$P_{k+1}(x_i) = \sum_{j'=1}^{N_k} \sum_{j''=1}^{N_k} p_{j'}^{(k)} p_{j''}^{(k)} Q_k(x_{j'}, x_{j''}, x_i), \quad (29)$$

where

$$p_j^{(k)} = \frac{y_k(x_j^{(k)})}{\sum_{i=1}^{N_k} y_k(x_i^{(k)})}. \quad (30)$$

5. If the stopping criterion is satisfied, then stop; otherwise, substitute $k + 1$ for k and go to Step 2.

4.2 Genetic Algorithm Behavior

The construction and evolution of the distributions $\{P_{k+1}\}$ provide considerable insights into the interplay of the procedural elements. This level of abstraction lies between those of the procedure and the populational transition operators of Markov chain analysis. Furthermore, it is useful for understanding how genetic algorithms search the feasible space and how they generate increasingly better candidate solutions. It is also suitable for rigorous mathematical analysis and derivation of convergence properties.

Genetic algorithms can be described on the basis of the three following heuristics, which are related to the procedural elements of genetic algorithms:

- i. the number of times a previous sample is chosen for constructing a transition probability, Q_k , is dependent on the function evaluation observed at that point,

- ii. the *similarities* between previous samples should be exploited in the construction of the transition probabilities, and
- iii. often enough, the objective or fitness function behaves similarly on *similar* samples.

The description of genetic algorithm behavior begins with a randomly generated set of samples from the search space (the initial population). For each sample, the objective function value is evaluated. Then pairs of high performance samples are competitively selected from the set of samples. For each pair of samples, another one or two new samples are randomly generated that are *similar* to the high performance samples. Since it is assumed that the objective function behaves similarly on similar samples, the new samples are also likely to be of high performance. The search process continues with the evaluation of the objective function at the new samples. Since the new samples also compete against each other in the selection process, the set of samples becomes increasingly concentrated in the high performance regions of the search space. As the samples become increasingly concentrated, they become more *similar* and the breadth of search dynamically decreases. Therefore, unlike most other global random search methods, genetic algorithms do not require predetermined schedules for controlling the construction of its sampling distributions.

The word *similar* is critical in the above description. However, there is no similarity criterion that applies to all problem domains and search spaces. While not yet properly investigated for this purpose, the *fitness correlation coefficient* of an operator may serve as a useful measure of similarity (Manderick, de Weger & Spiessens, 1991). The similarities exploited by an algorithm may be either genotypic or phenotypic, depending on the nature of the implementation. In the canonical genetic algorithm, it is the similarities in the candidate solution encodings that are exploited. Each of the traditional crossover operators (*i.e.*, one-point, multi-point, uniform, and parameterized uniform crossover) preserves the portions or bits of the encodings common to both *parents* in the children. Searching is performed by exchanging or randomizing the remaining bits in some manner. Since the

likelihood of altering bits of the candidate solution encoding through the process of mutation typically decreases exponentially with the number of altered bits, mutation also results in encodings that are similar to the original encoding. Interestingly, it is in this manner that the string similarities common to high performance samples pervade later populations. A more extensive explanation for observations of schema growth that does not appeal to the schema theory is presented in (Peck, 1993, §5.4).

In addition to considering the satisfaction of the second heuristic, we will now consider the other heuristics as well. In genetic algorithms, the first heuristic is satisfied by the global sampling phase, which is described by (24). The third heuristic is problem dependent. As addressed in Subsection 5.1, it is also dependent on the candidate solution representation. Furthermore, it has been pointed out that the genetic algorithm will degenerate into a random search if this heuristic is not satisfied (Rawlins, 1991).

4.3 The Sufficiency of the Theory

The mathematical description of the theory presented in this section is an exact representation of genetic algorithms based on the procedural elements. Thus, any phenomena of genetic algorithms will be explainable in its context. The explanatory and predictive capabilities of the theory are drawn upon throughout the remainder of this paper. The theory is also robust with respect to algorithmic variations. Procedure 5, for example, allows for fitness scaling, ranking, non-traditional recombination operators, independence of the encoding method, and arbitrary search spaces. Consequently, this theory is sufficient according to the criteria established at the beginning of Section 2.

Since both this theory and the theory presented in (Vose & Liepins, 1991a; Nix & Vose, 1992; Vose, 1993a) are exact, they are isomorphic. Since they have different theoretical bases and levels of abstraction, however, these two analytical perspectives should be complementary. These theories are distinguished from each other in two ways. The first is a change of emphasis or interpretation. In (Vose & Liepins, 1991a; Nix & Vose, 1992; Vose, 1993a), the

interpretation of the mathematics is lumped into a transition between populations. In the present theory, the emphasis is on how the components of the sampling distribution affect the search. The second distinguishing characteristic is the consideration of the phenotypic sampling distribution, if possible.

5 Factors Affecting the Sampling Distributions

Based on the conclusions of Section 4.2, understanding the factors affecting the sampling distributions $\{P_{k+1}\}$ is particularly important for understanding, applying, and designing genetic algorithms. In pursuit of this understanding, this section addresses the issues associated with the encoding of candidate solutions, the construction of the sampling distributions R_k (*i.e.*, selection), the construction of the distributions Q_k (*i.e.*, recombination), and population management.

5.1 Candidate Solution Encoding

Genetic algorithms work by exploiting *similarities* between previous samples and they depend on the objective function behaving similarly on *similar* samples. A crucial design issue, therefore, is the choice of similarities to exploit. Ideally, these similarities should be chosen with respect to the nature of the candidate solutions and the problem under consideration.

Typically, genetic algorithms encode candidate solutions and then exploit the similarities in the encodings. As a consequence, the choice of candidate solution encoding has a tremendous impact on the performance of genetic algorithms. According to the choice of encoding, a problem may be reduced to the archtypically easy “counting 1’s” problem (Vose & Liepins, 1991b), or genetic search may be rendered no more effective than a pure random search (Rawlins, 1991).

For greatest benefit, the encoding method should be matched to the candidate solutions and the problem under consideration such that similar strings will result in similar candidate solutions. Unfortunately, it is not generally possible to preserve similarities in both \mathcal{A} and

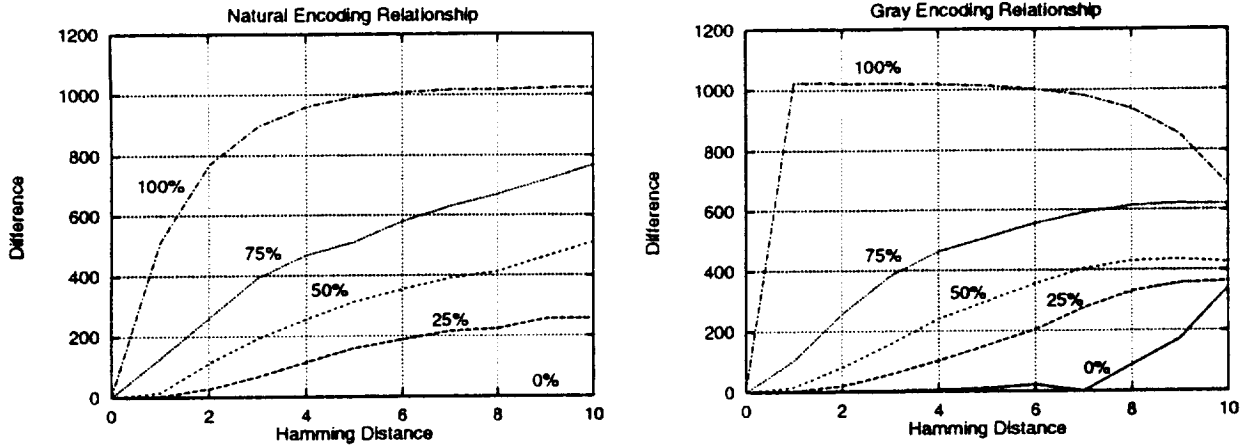


Figure 1: The relationship between the similarities of encodings and the similarities of the numbers they represent: *left*) when natural code is used, *right*) when gray code is used.

\mathcal{X} . Typically, genetic algorithm practitioners simply rely upon the fortuitous existence of exploitable similarities. Since the use of binary encodings increases the number of opportunities for exploitable similarities, it is not surprising that such encodings are the most commonly used.

To illustrate the problems of choosing an encoding, the specific problem of encoding an integer is considered in (Peck, 1993). Both natural code and the gray code used in Genesis Version 5.0 (Grefenstette, 1990) are analyzed. Ten bit encodings were used to represent integers in the range $[0,1023]$. In this analysis, the Hamming distance and the absolute difference are used as similarity measures for the encodings and integer values, respectively. As shown in Figure 1, two similar encodings will not necessarily result in similar integers for either encoding method. In fact, no integer encoding longer than two bits can satisfy this objective. This is because an integer is adjacent to only two other integers, yet an integer encoded with ℓ bits, is a Hamming distance of one from exactly ℓ other encodings. Figure 1 also suggests why genetic algorithms using these encodings are usually effective. The region between the 25th and 75th percentiles in each case shows that, in most instances, increasingly similar encodings result in increasingly similar integers.

The above discussion illustrates that it is very difficult to design an appropriate candidate solution encoding scheme, even when the candidate solution is as simple as an integer. It is

also very difficult to envision the distribution of candidate solutions across \mathcal{A} . This difficulty, combined with trying to understand how \mathcal{A} is being sampled by selection and recombination, makes it very difficult to understand genetic algorithm behavior in either the genospace or the domain of the problem being considered.

The many problems associated with encoding the candidate solutions and designing the sampling distributions to exploit string encoding similarities may very easily be eliminated by simply designing the sampling distributions to exploit similarities in the candidate solutions themselves. There is no theoretical requirement for the use of string encodings and there are many advantages to their elimination:

1. The problem specific structure of \mathcal{X} is typically much better understood than the distribution of candidate solutions across \mathcal{A} .
2. The recombination operators, Q_k , may be customized to exploit knowledge of the structure and similarities of the candidate solutions that are pertinent to the problem under consideration.
3. The behavior of the genetic algorithm will be better understood since the relationship of the sampling distributions to the structure of \mathcal{X} will be better understood.
4. Only the recombination operators are problem dependent, the remainder of the algorithm (Procedure 5) is unchanged.
5. Mathematical analysis is easier due to the elimination of the mapping \mathcal{M} .

Finally, it should be noted that designing genetic algorithms to search the phenospace, \mathcal{X} , as opposed to the genospace, \mathcal{A} , is already a common practice (*e.g.*, consider order dependent problems).

Radcliffe has also considered many of these ideas (Radcliffe, 1991b; Radcliffe, 1991a; Radcliffe, 1993). Referring to subsets of the search space as equivalence classes or formae, Radcliffe argues:

The critical tasks are thus finding formae which characterise solutions in meaningful ways and developing operators which usefully manipulate these formae (Radcliffe, 1991b).

These formae are generalizations of schemata that are not necessarily defined with respect to string similarities. By considering recombination operators that characterize solutions in *meaningful ways* and do not necessarily exploit string similarities, the need for string encodings is effectively eliminated.

5.2 The R_k Class of Distributions: Selection

The distributions R_k in (27) make use of global information obtained about the objective function f . Furthermore, these distributions are largely responsible for concentrating search in high performance regions of the search space. Since the realizations obtained by sampling the distributions R_k are previously obtained samples of \mathcal{X} , these distributions do not generate new candidate solutions or expand the search domain.

To a great degree, the way of constructing the distributions R_k establishes the general structure and originality of a global random search method (Zhigljavsky, 1991). In the canonical genetic algorithm, proportional selection is used, as in (1). In practice, auxiliary functions f_k related to the objective function f are typically constructed for the purposes of fitness scaling or ranking. The distributions R_k are then implemented according to (30). Many other methods may be used instead of proportional selection (Goldberg & Deb, 1991; Bäck & Hoffmeister, 1991; de la Maza & Tidor, 1993), including the methods used in evolution strategies (Bäck & Schwefel, 1993; Bäck, Hoffmeister & Schwefel, 1991) and evolutionary programming (Fogel & Atmar, 1990; Bäck & Schwefel, 1993).

Proportional selection is very simple, is suitable for use in the presence of noise, and it has nice theoretical properties. Theorem 3 indicates that the the best string in the initial population eventually dominates the population (Peck, 1993; Peck & Dhawan, 1993). This theorem simulates the effects of an arbitrarily large population by allowing fractional numbers

of individuals. Comparing (31) to (22) provides additional insights into genetic algorithm behavior. These equations are consistent with Equations (7) and (8) of (Goldberg & Deb, 1991).

Theorem 3 *The observed average population fitness, $\bar{f}(\mathbf{A}(t))$, at time t , and the number of instances of a particular string A_i at time t , $m(A_i, t)$, resulting from the use of proportional selection may be expressed:*

$$\bar{f}(\mathbf{A}(t)) = \frac{\sum_{A_i \in \mathcal{A}} m(A_i, 0) f^{t+1}(A_i)}{\sum_{A_j \in \mathcal{A}} m(A_j, 0) f^t(A_j)}, \quad (31)$$

and

$$m(A_i, t) = \frac{N m(A_i, 0) f^t(A_i)}{\sum_{A_j \in \mathcal{A}} m(A_j, 0) f^t(A_j)}, \quad (32)$$

where N denotes the size of the population, and $m(A_j, 0) = 0$ if $A_j \notin \mathbf{A}(0)$.

Proof: The following inductive proof begins with the initial steps. By definition,

$$m(A_i, 0) = \frac{N m(A_i, 0) f^0(A_i)}{\sum_{A_j \in \mathcal{A}} m(A_j, 0) f^0(A_j)}, \quad (33)$$

and

$$\bar{f}(\mathbf{A}(0)) = \frac{1}{N} \sum_{A_i \in \mathcal{A}} m(A_i, 0) f(A_i), \quad (34)$$

$$= \frac{\sum_{A_i \in \mathcal{A}} m(A_i, 0) f^1(A_i)}{\sum_{A_j \in \mathcal{A}} m(A_j, 0) f^0(A_j)}, \quad (35)$$

since $\forall t \geq 0, N = \sum_{A_i \in \mathcal{A}} m(A_i, t)$. Furthermore,

$$m(A_i, 1) = \frac{m(A_i, 0) f(A_i)}{\bar{f}(\mathbf{A}(0))}, \quad (36)$$

$$= \frac{m(A_i, 0) f^1(A_i)}{\frac{1}{N} \sum_{A_j \in \mathcal{A}} m(A_j, 0) f^1(A_j)}, \quad (37)$$

$$= \frac{N m(A_i, 0) f^1(A_i)}{\sum_{A_j \in \mathcal{A}} m(A_j, 0) f^1(A_j)}, \quad (38)$$

and

$$\bar{f}(\mathbf{A}(1)) = \frac{1}{N} \sum_{A_i \in \mathcal{A}} m(A_i, 1) f(A_i), \quad (39)$$

$$= \frac{1}{N} \frac{\sum_{A_i \in \mathcal{A}} N m(A_i, 0) f(A_i) f(A_i)}{\sum_{A_j \in \mathcal{A}} m(A_j, 0) f^1(A_j)}, \quad (40)$$

$$= \frac{\sum_{A_i \in \mathcal{A}} m(A_i, 0) f^2(A_i)}{\sum_{A_j \in \mathcal{A}} m(A_j, 0) f^1(A_j)}. \quad (41)$$

Let us now assume that

$$m(A_i, k) = \frac{N m(A_i, 0) f^k(A_i)}{\sum_{A_j \in \mathcal{A}} m(A_j, 0) f^k(A_j)} \quad (42)$$

and

$$\bar{f}(\mathbf{A}(k)) = \frac{\sum_{A_i \in \mathcal{A}} m(A_i, 0) f^{k+1}(A_i)}{\sum_{A_j \in \mathcal{A}} m(A_j, 0) f^k(A_j)}. \quad (43)$$

Then

$$m(A_i, k+1) = \frac{m(A_i, k) f(A_i)}{\bar{f}(\mathbf{A}(k))}, \quad (44)$$

$$= m(A_i, k) f(A_i) \frac{1}{\bar{f}(\mathbf{A}(k))}, \quad (45)$$

$$= \frac{N m(A_i, 0) f^k(A_i) f(A_i)}{\sum_{A_j \in \mathcal{A}} m(A_j, 0) f^k(A_j)} \cdot \frac{\sum_{A_j \in \mathcal{A}} m(A_j, 0) f^k(A_j)}{\sum_{A_{j'} \in \mathcal{A}} m(A_{j'}, 0) f^{k+1}(A_{j'})}, \quad (46)$$

$$= \frac{N m(A_i, 0) f^{k+1}(A_i)}{\sum_{A_j \in \mathcal{A}} m(A_j, 0) f^{k+1}(A_j)}, \quad (47)$$

and

$$\bar{f}(\mathbf{A}(k+1)) = \frac{1}{N} \sum_{A_i \in \mathcal{A}} m(A_i, k+1) f(A_i), \quad (48)$$

$$= \frac{1}{N} \frac{\sum_{A_i \in \mathcal{A}} N m(A_i, 0) f^{k+1}(A_i) f(A_i)}{\sum_{A_j \in \mathcal{A}} m(A_j, 0) f^{k+1}(A_j)}, \quad (49)$$

$$= \frac{\sum_{A_i \in \mathcal{A}} m(A_i, 0) f^{k+2}(A_i)}{\sum_{A_j \in \mathcal{A}} m(A_j, 0) f^{k+1}(A_j)}. \quad (50)$$

Since it has been shown that the theorem is satisfied for $t = 0, 1$ and that if the theorem

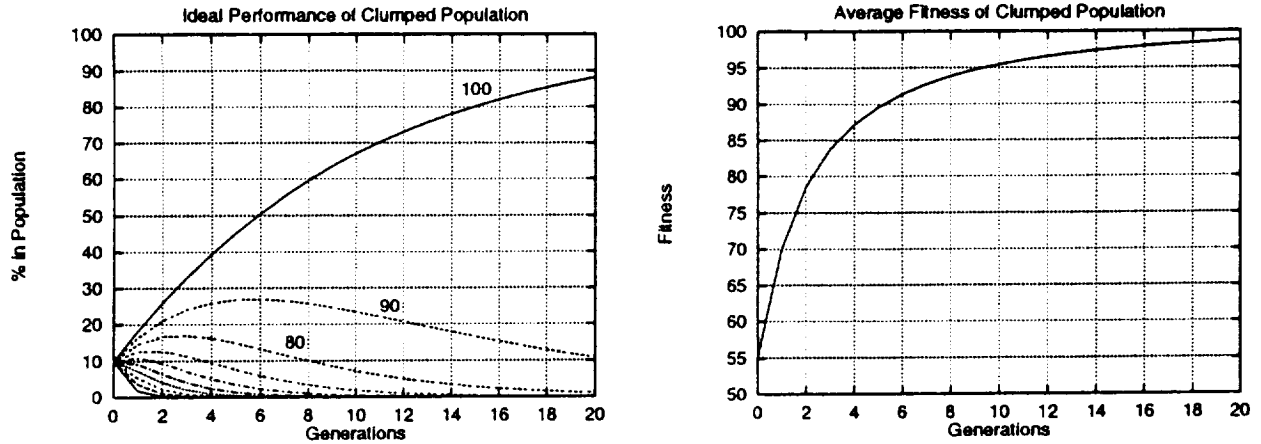


Figure 2: Ideal string and population fitness growth curves, based on a clumped initial population: *left*) The growth of instances of the strings having the indicated fitness, *right*) The growth of the observed average population fitness.

is satisfied at $t = k$ then it is also satisfied at $t = k + 1$, the process of induction completes the proof. ■

In (Syswerda, 1991), the effects of proportional selection on the growth of strings are investigated. Three cases are considered: the ideal (infinite population) case, the finite population case using the standard ‘roulette wheel’ proportional selection method, and the finite population case using a selection variance reduction technique, Stochastic Universal Sampling (SUS) selection method (Baker, 1987). In all three cases, the population fitnesses are initially clumped at specific values: 10% of the population has a fitness of 10, 10% has a fitness of 20, and so on, up to a fitness of 100. A number of interesting observations can be made from the presented results. In the ideal case, the growth curves, which were obtained using difference equations, are indistinguishable from those obtained using the equations of Theorem 3. The growth curves derived from Theorem 3 are presented in Figure 2. When a finite population and standard selection are used, the growth curves are nearly ideal, but noticeably different. When the variance reduction technique is employed, the growth curves are indistinguishable from the ideal curves.

In (Peck, 1993), an empirical study is performed to determine whether the discrepancy between the ideal growth curves and the growth curves using the finite population and stan-

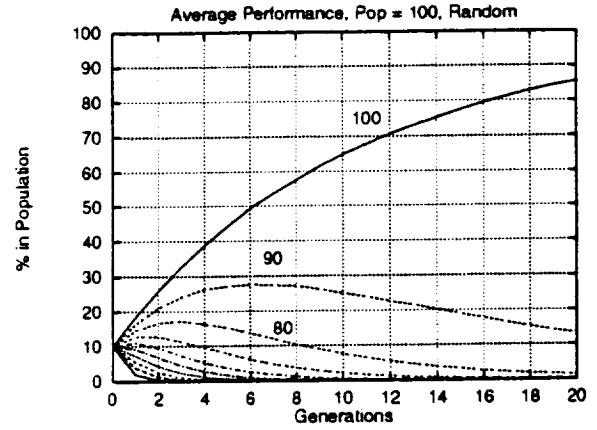
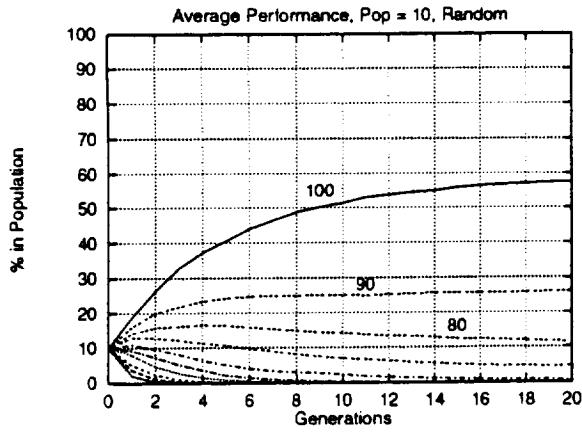


Figure 3: The average proportion of individuals of different fitnesses, using standard proportional selection, in clumped population distributions of *left*) 10 individuals, and *right*) 100 individuals.

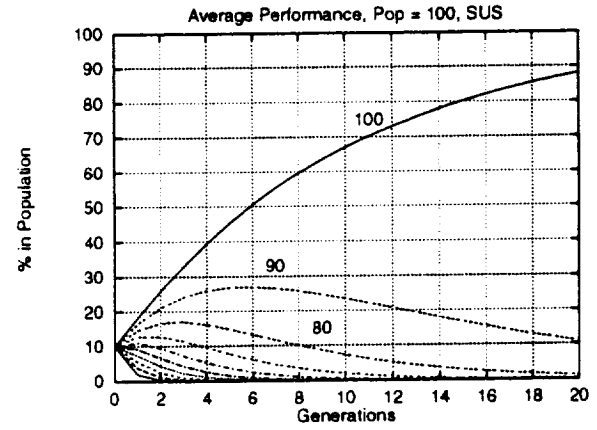
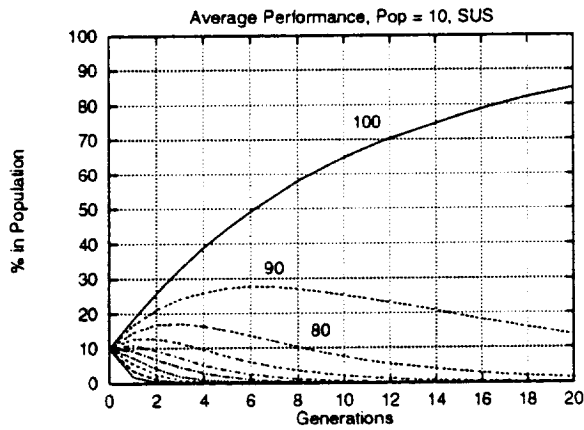


Figure 4: The average proportion of individuals of different fitnesses, using SUS proportional selection, in clumped population distributions of *left*) 10 individuals, and *right*) 100 individuals.

standard selection is significant. Populations of 10, 20, 40, and 100 strings were investigated. Uncertainty in the results was reduced by averaging the curves from 1000 independent experiments. Both standard and SUS proportional selection methods were investigated to determine the effects of selection noise. Figures 3 and 4 present a portion of the results.

The empirical results indicate that poorer performance should be expected when smaller populations are used, regardless of the selection method. Analytical proofs or explanations of this observation are presently unavailable. Using standard proportional selection, extinction of the best individuals was observed for populations of 10, 20, 40, and 100 individuals

in 40%, 20%, 3%, and 0% of the trials, respectively. Extinction of the best individuals is not possible using SUS proportional selection. Extinction, therefore, can explain some of the poorer performance, but not all of it. The poorer performance does seem to be well correlated with the sampling variance, however. There is higher sampling variance for the smaller populations and the performance is worse for smaller populations, regardless of the selection method. Furthermore, the use of the variance reduction technique results in improved performance. Unfortunately, the relationship, if any, between high sampling variance and poorer selection performance is presently not understood.

5.3 The Q_k Class of Distributions: Recombination

The distributions Q_k in (27) typically perform a localized search according to some similarity measure, and are referred to as recombination operators in the genetic algorithm literature. The distributions $Q_k(z', z'', \cdot)$ are dependent on two realizations, z' and z'' , which are likely to be of high performance since they are obtained through selection. These distributions are typically designed to exploit similarities between these two high performance realizations. These distributions can also be designed to exploit inferences about the local behavior of the objective function f based on the two samples, z' and z'' , and their evaluations (Peck, 1993). The dependence of the distributions $Q_k(z', z'', \cdot)$ on two samples combined with the use of selection¹ can eliminate the need for scheduling the narrowing of local search, which is required for most adaptive global random search methods (*e.g.*, the simulated annealing and the methods of generations (Zhigljavsky, 1991)). Since this is typically done in genetic algorithms, both the distributions R_k and the distributions Q_k are typically adapted on the basis of information obtained during the search.

In Section 4, it is argued that genetic algorithm behavior can best be understood by understanding the sampling distributions induced on the phenospace. Accordingly, the sampling distributions imposed on \mathbb{R}^n by the traditional recombination operators will now be

¹Recall that selection, or the sampling of the distributions R_k , concentrates the sampling distribution in the high performance regions observed globally.

considered with the use of a novel visualization technique. The operators that will be characterized are one-point crossover and uniform crossover. Other traditional recombination operators are visualized in (Peck, 1993). Due to the independence of the encoded parameters it is sufficient to consider the sampling of one dimension at a time, \mathbb{R}^1 . However, due to the dualism between encodings and recombination operators (Battle & Vose, 1991; Vose & Liepins, 1991b), visualizations will be presented of the recombination operators applied to both natural code and the gray code used in Genesis Version 5.0 (Grefenstette, 1990). Finally, as is typically the case, the real values will actually be encoded as integers and used as a real value by applying an affine transformation.

The objective of this visualization technique is to communicate where the realizations of the recombination operators, $Q_k(z', z'', \cdot)$, are likely to be obtained relative to the location of the parents, z' and z'' . To fulfill this objective, all integers are encoded using six bits, and it is assumed that all pairs of parents are equally likely. For a particular pair of parent values, it is possible to compute the likelihood of realizing particular values given the recombination operator and the encoding scheme. A suitable visualization can be constructed by accumulating the marginal sampling distributions for sets of parent values separated by a given distance. To properly accumulate these distributions, they are translated by the amount required to position the mean of the two parents on the center column of the image². Each marginal distribution is then used to construct a single row of the visualization, where the brightest pixel values correspond to the most likely realizations. The top row of the resulting image corresponds to the marginal sampling distribution of parents separated by a distance of zero (they are the same). Successive rows correspond to the marginal distributions of increasingly separated parents. Finally, the bottom row corresponds to the marginal distribution of parents separated by a distance of 63. As shown in (Peck, 1993), it is also insightful to visualize the feasible realizations by setting all locations with a positive probability of being

²The image requires a minimum of 127 columns because when both parents are 0, the marginal sampling distribution occupies columns 63–126, and when they are both 63, the marginal sampling distribution occupies columns 0–63. For all other combinations of parents, the marginal distributions fall into this range of columns.

realized to white, and all other locations to black.

Figure 5 shows the sampling distribution resulting from the application of one-point and uniform crossover to integers encoded with 6-bit natural code. Figure 6 presents the visualizations resulting from the use of 6-bit gray code. These visualizations indicate that the distributions generated by one-point crossover are more concentrated in the vicinity of the parents than those resulting from uniform crossover. The salient characteristic of the sampling distributions resulting from the use of the gray code representation is that the breadth of search decreases as the distance between the parents decreases.

In (Peck, 1993), one-point, two-point, uniform, and parameterized uniform crossover operators using both natural and gray encodings are applied to De Jong’s test suite (De Jong, 1975), and their effectiveness is compared on the basis of five performance measures. It is found that those operators that tend to sample most often near the parents result in superior performance. Therefore, it may be concluded that concentrating and constraining search in the vicinity of the parents results in superior performance. This conclusion is further bolstered by the recommended settings of the recombination control parameters, such as crossover and mutation probabilities, which serve to further localize search. Finally, this conclusion has been favorably exploited in the design of a family of recombination operators for use when $\mathcal{X} \subset \mathbb{R}^n$ (Peck, 1993). An example of these operators and its visualization are presented in (52) and Figure 9, respectively.

5.4 Management of the Population

The population is the basis for the construction of the sampling distributions. The information obtained by the genetic algorithm up to a certain iteration is entirely contained in the distribution of the population’s samples and in the evaluations of the objective function obtained at those samples. In fact, this information completely determines the distributions R_k . For this reason, it is arguable that the management of the population should have been discussed in Subsection 5.2. However, for the sake of clarity, the many issues associated with

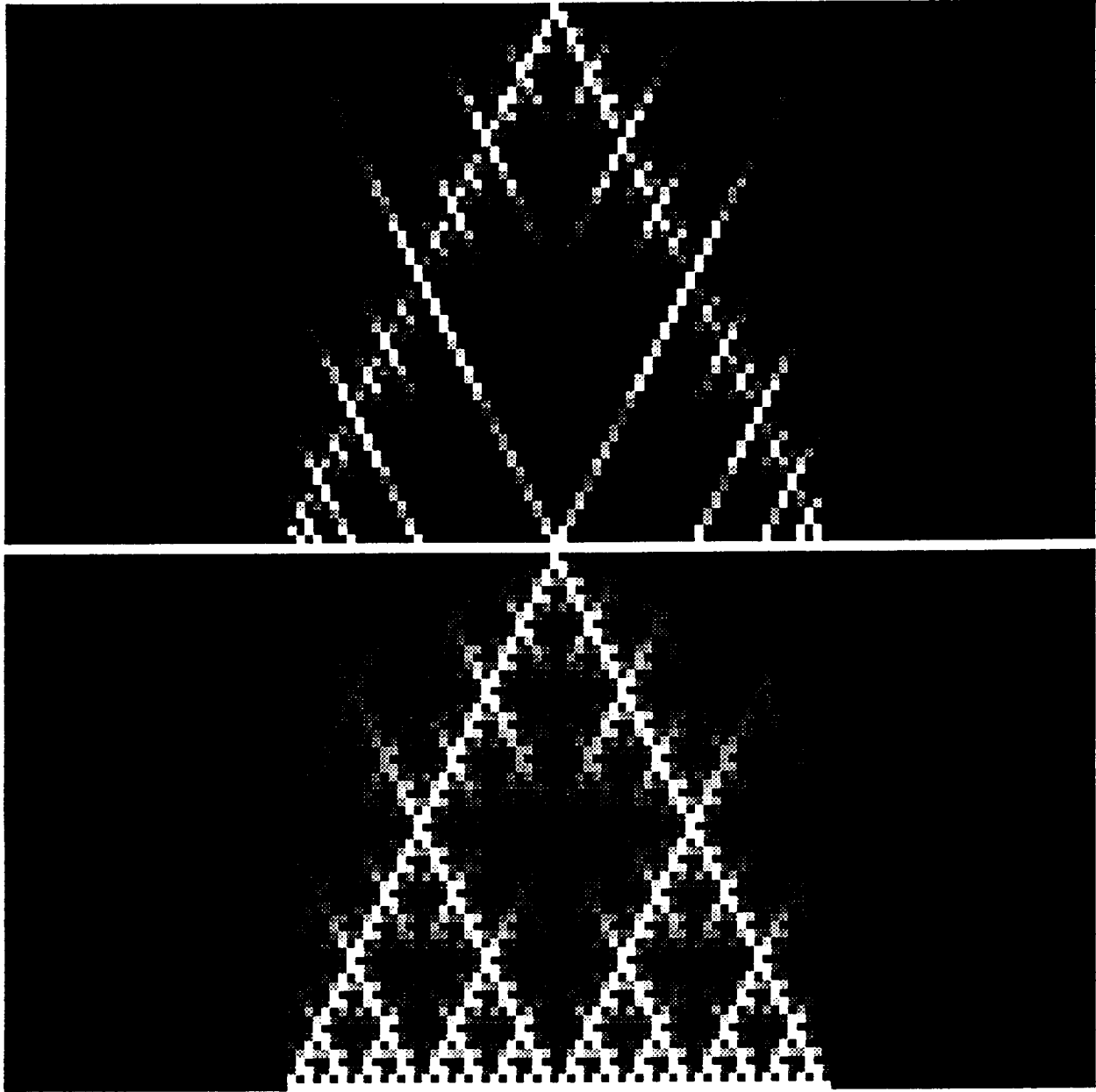


Figure 5: Sampling distributions of one-point and uniform crossover search in the real domain with natural code representations: *top*) one-point crossover, *bottom*) uniform crossover.

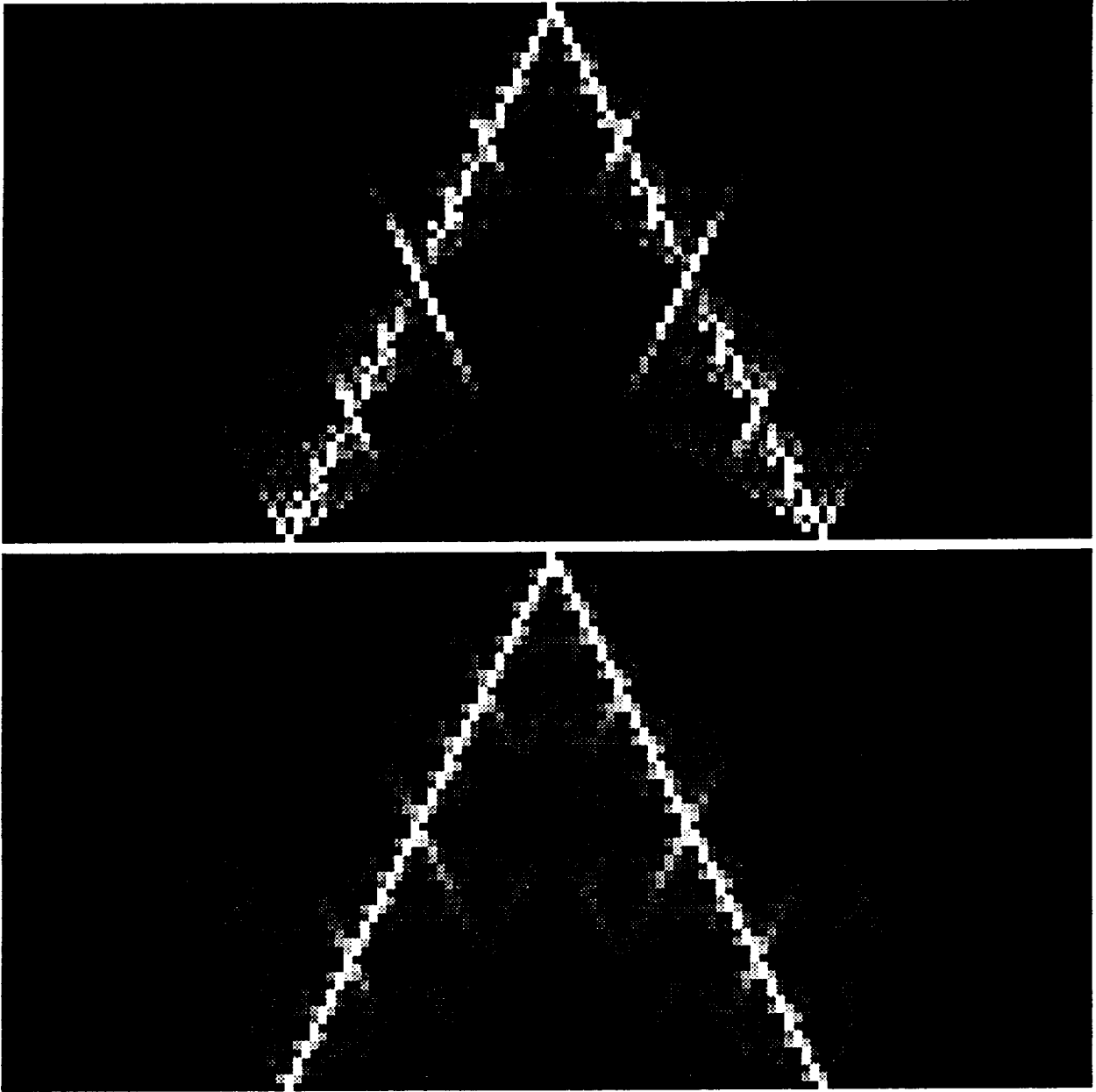


Figure 6: Sampling distributions of one-point and uniform crossover search in the real domain with gray code representations: *top*) one-point crossover, *bottom*) uniform crossover.

the management of the population are considered here separately. The issues considered are those associated with the composition and creation of the population, the updating of the population, and the deletion of members from the population.

5.4.1 Population Issues

Of the two population issues considered in this subsection, population sizing and initialization, population sizing is certainly the most thoroughly investigated in the literature. The population provides an estimate of the objective function behavior. Obviously, a larger population results in a more dense sampling of the objective function and a better estimate. If the objective is to ensure with a certain degree of confidence that the algorithm will adequately search the objective function, then the complexity of the phenospace and the characteristics of the objective function should be considered in the sizing of the population. If the function varies significantly in small regions, then a larger population will be necessary to provide an effective estimate, whereas a slowly varying function may be adequately estimated with very few samples. Similarly, a highly complex phenospace will require more samples, than a very simple one. The drawback to the use of larger populations is that the rate of improvement or convergence is slower when measured by the number of evaluations performed.

The population sizing problem has been considered in the literature both empirically (De Jong, 1975; Grefenstette, 1986; Schaffer, Caruana, Eshelman & Das, 1989; Jog, Suh & Gucht, 1989) and analytically (Goldberg, 1989b; Reeves, 1993; Goldberg & Rudnick, 1988; Goldberg, Deb & Clark, 1992; Goldberg, Deb & Clark, 1993). The empirical studies have suggested populations ranging from 20–200, depending on the optimality criterion. Of the analytical approaches, information about the objective function is considered only in (Goldberg & Rudnick, 1988; Goldberg, Deb & Clark, 1992; Goldberg, Deb & Clark, 1993), albeit in the form of collateral noise. The favorable empirical results obtained with these methods might be explainable in terms of the objective function, the properties of the phenospace, and the relationship between the schemata and the phenospace. If so, they may provide the basis for population sizing methods that are based more directly on the first two properties. Such a

method would also be applicable when binary encodings of the candidate solutions are not used.

A population management issue that has received little attention in the literature is improving population initialization. This literature is reviewed in (Peck, 1993), and a novel initialization technique based on stratified sampling is proposed. This method is motivated by the facts that reducing randomness can increase efficiency, and stratified sampling has been shown to dominate independent sampling (Zhigljavsky, 1991, §4.4). Stratified sampling involves dividing the sampling region, \mathcal{X} , into m subregions of equal volume. Then, if $N = m\ell$ samples are desired, each of the m subregions is randomly sampled ℓ times, using a uniform distribution. The effects of stratified initialization on genetic algorithm behavior, however, are negligible when applied to De Jong's test suite using an initial population of 50 samples. This suggests that genetic algorithm behavior is robust with respect to slight variations of the initial population, which is desirable. Problems for which \mathcal{X} or f is highly complex, or only a small initial population is possible, may benefit from stratified initialization.

5.4.2 Sequentiality and Deletion

Genetic algorithms adapt their sampling distributions based on information acquired during the search. Most commonly, the sampling distributions $\{P_{k+1}\}$ are sampled N times before they are updated, where N is the size of the population. In *sequential* or *steady-state* variants, the sampling distributions are updated more frequently, such as after each sample. This makes it possible to exploit information sooner after it is acquired. The portion of the population that is replaced prior to updating the sampling distributions is described by the *generation gap*.

Increased sequentiality results in increased selection noise or variance compared to the use of generational replacement and the use of sampling variance reduction techniques, such as SUS selection (Baker, 1987). Baker's "Stochastic Universal Sampling" technique (Baker, 1987). Sampling variance reduction techniques work by establishing codependencies among

the realizations of R_k . The more samples there are to be obtained from R_k , the more effective the sampling variance reduction technique will be. Selection variance is increased with the degree of sequentiality because fewer samples from R_k are obtained at a time. Some of these assertions are supported in the literature. It has been concluded based on the use of *uniform* or *random* deletion that the potential advantages of overlapping populations are dominated by the negative effects of genetic drift or allele loss (De Jong, 1975; De Jong & Sarma, 1993). In (De Jong & Sarma, 1993), it is concluded that the higher variance associated with smaller generation gaps leads to greater variation of actual growth curves of individuals on a single genetic algorithm run, and more genetic drift or allele loss.

Aside from the negative effects of increased selection noise, the performance of sequential genetic algorithms is predominately determined by the deletion method. Consider the following strategies for removing samples from the current population to allow for the insertion of new samples. Best-in-first-out (BIFO) deletion, in which the best observed sample in the population is the first removed, would clearly result in a counterproductive influence on behavior. Conversely, worst-in-first-out (WIFO) deletion exploits observations very aggressively to concentrate samples in the highest performance regions encountered. Finally, last-in-first-out (LIFO) deletion would degenerate into a non-uniform random search with a very weak adaptive element, which is the last sample. Only WIFO deletion is in common use.

In (De Jong & Sarma, 1993), the effects of the generation gap on performance are investigated. It is concluded that the growth curves of genetic algorithm selection are independent of the generation gap, and there is no compounding effect (De Jong & Sarma, 1993). These conclusions are based on the use of uniform deletion, the comparison of the ideal growth curves for generational genetic algorithms and steady-state genetic algorithms with uniform deletion, which are presented in (Syswerda, 1991), and on mathematical analysis. Uniform deletion, however, is not an aggressive deletion method. Furthermore, it has been shown that steady-state genetic algorithms with uniform deletion are not actually identical

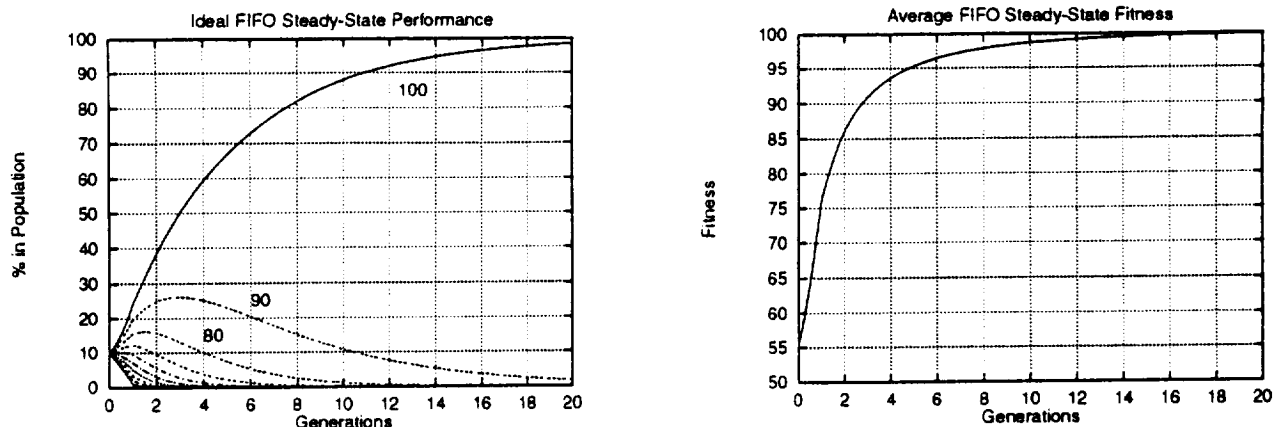


Figure 7: The ideal behavior of steady-state proportional selection with FIFO deletion, applied to the clumped population distribution: *left*) the average proportion of individuals of different fitnesses in the population, *right*) the average population fitness.

to generational genetic algorithms (Peck, 1993). Conversely, advantages can be accrued from sequentiality. These advantages, illustrated by the use of first-in-first-out (FIFO) deletion applied to a sequential genetic algorithm, may be seen by comparing Figures 2 and 7.

Many methods for deletion have been proposed for use in genetic algorithms (Syswerda, 1991). These methods may be distinguished by whether the deletion strategy makes use of observed sample evaluations. Methods that do not use fitness evaluations, such as uniform and FIFO deletion, are preferred when the objective function is evaluated with noise since they will not result in a population biased by samples evaluated with favorable noise³. Conversely, those methods that use fitness information, can have more aggressive exploitation, but they are not suitable for use in the presence of noise. To avoid premature convergence, however, care must be taken to ensure that Theorem 1 is not violated.

6 Convergence Properties

In this section, the convergence properties of genetic algorithms will be considered. First, a property of genetic algorithms that makes global convergence proofs difficult, if not impossible, will be discussed. Subsequently, a simplistic remedy will then be provided. This remedy

³The effects of noise on genetic algorithms are carefully examined in (Peck, 1993, §7.2).

will be accompanied by proofs of convergence to global optima.

6.1 Why Genetic Algorithms may not Converge

While genetic algorithms satisfy Zhigljavsky’s requirements on the global sampling components, they do not satisfy the requirements on the local sampling components. As discussed previously, the sampling distributions of the recombination operators are constrained locally by the *similarities* of the two parent samples. However, the parents are chosen by a global sampling component. Therefore, the two parents may not be very similar. As a result, the recombination sampling distributions may not be adequately constrained or localized for convergence.

The dependence of the local sampling distributions on two samples can have undesirable consequences, such as convergence to sub-optima and divergent behavior. To illustrate these effects, consider the following function with the feasible space $\mathcal{X} = x : x \in [0, 1]$:

$$F6_\alpha(x) = -\left(x^8 + x - 1\right)^4 + \left(x^8 + x - 1\right)^2 + \alpha x. \quad (51)$$

This function is illustrated in Figure 8 for values of α equal to 0.22 and 0.23, respectively. This function has an optimum at approximately 0.96 with a narrow peak and a sub-optimal local maximum at approximately 0.35 with a broad peak. This function was designed such that a recombination event between samples from each peak will result in a disproportionate number of realizations in the larger, sub-optimal peak, and a recombination event between samples from the same peak will likely result in realizations within the same peak.

If the breadth of the sampling distributions Q_k is dependent on the distance between the parents, then it is expected that a sampling distribution tug-of-war will ensue between the large, sub-optimal mass and the smaller, higher performance mass. Selection will always favor the samples within the optimal peak. Thus, if recombination always resulted in a realization occurring on the peak of the parent sample around which Q_k is centered, then selection would concentrate the population on the optimal peak. In this manner, samples may be *stolen* by the optimal peak from the sub-optimal peak. However, samples within the

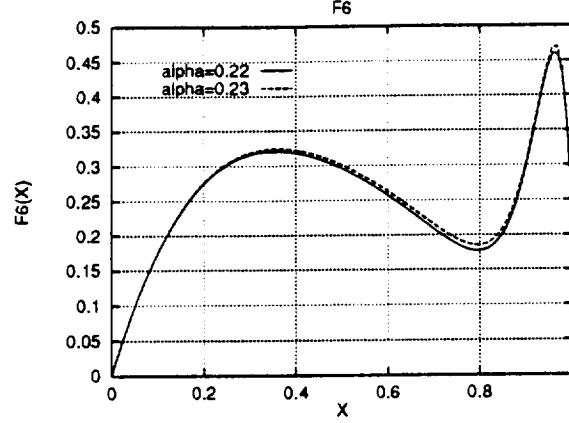


Figure 8: An illustration of $F6$ in the feasible space $\mathcal{X} = x : x \in [0, 1)$ for $\alpha = 0.22, 0.23$.

sub-optimal peak will also be selected with positive probability. Due to the nature of $F6$, realizations of Q_k centered at a sample within the optimal peak will often be obtained on the sub-optimal peak when the other parent sample is from the sub-optimal peak. If such a realization is then recombined with another sample from the sub-optimal peak, then the resulting sample will likely also be on the sub-optimal peak. In this manner, samples may be *stolen* from the optimal peak by the sub-optimal peak. Loosely speaking, if the rate at which samples are stolen from one peak to the other is exactly balanced by the other peak, then a steady state distribution or eigen-measure will occur. This situation would be unstable since a perturbation in the distribution will favor one peak or the other, which would be further reinforced by selection.

To test the behavior of the genetic algorithm on this function, one of the three basic recombination operators proposed in (Peck, 1993) was used. The recombination operator is applied to each dimension independently. The basic form of its density is

$$q(z', z'', x) = \frac{1}{2\omega} \varphi\left(\frac{(x - z')}{\omega}\right) + \frac{1}{2\omega} \varphi\left(\frac{(x - z'')}{\omega}\right), \quad (52)$$

where $\varphi(x)$ is an arbitrary symmetric density centered at zero, $\omega = \kappa|z' - z''|$, and κ is a control parameter. Densities of this form are constructed directly from the candidate solutions, are centered around each parent, and the search breadth is proportional to the distance between the parents. The concentration of the density around the parents can be

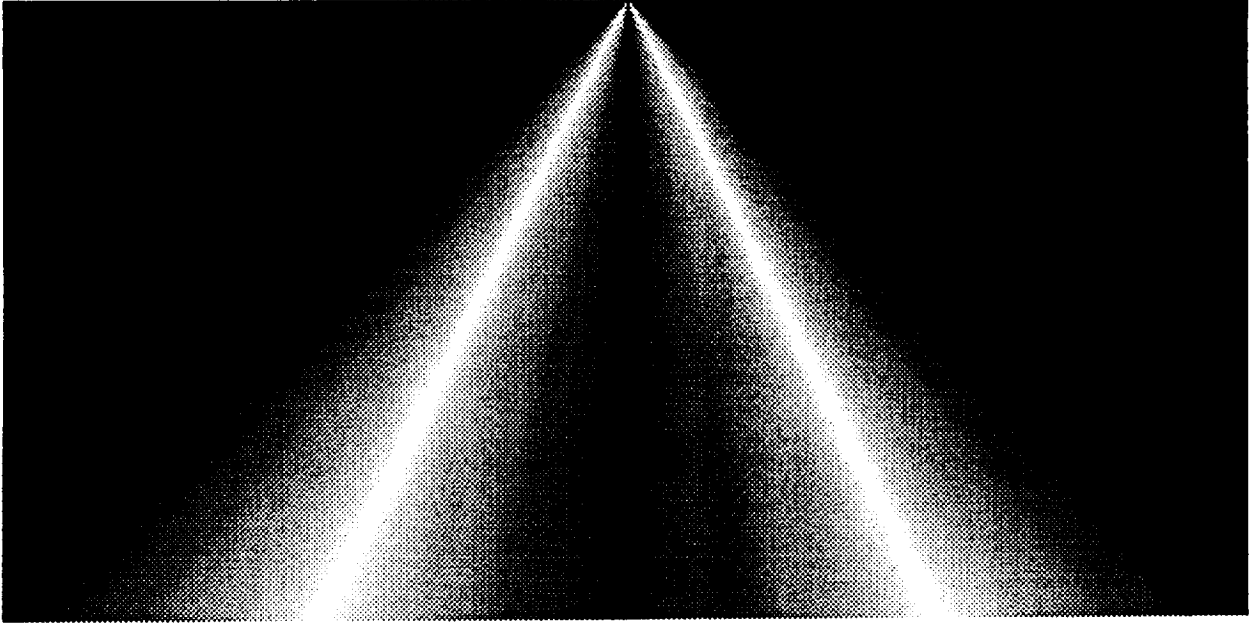


Figure 9: The sampling distribution of the triangular recombination operator with a base of width 1.0.

controlled by varying κ . In (Peck, 1993), $\varphi(x)$ is set to the Gaussian density, the triangular or roof density, and the uniform density. In this case, however, $\varphi(x) = t(x)$, where $t(x)$ is the triangular density with zero mean and a base width of $\kappa = 1.0$. A realization, r , of $t(x)$ may be obtained from a realization, ξ , of a uniform deviate on the range $[0, 1)$ according to

$$r(\xi) = \begin{cases} \frac{1}{2} (-1 + \sqrt{2\xi}) & \text{if } \xi < 0.5 \\ \frac{1}{2} (1 - \sqrt{2 - 2\xi}) & \text{if } \xi \geq 0.5. \end{cases}$$

The visualization of the resulting sampling distribution is provided in Figure 9.

To avoid premature convergence due to inadequate sampling and to reduce the stochastic effects, a population of 10,000 samples was used. This population was initialized by sampling a uniform distribution on the unit interval. Figure 10 shows the progression of sampling distributions for $\alpha = 0.22$ and $\alpha = 0.23$. It was found that for values of $\alpha \leq 0.22$ the sampling distributions will converge to the sub-optimal peak. It was also found that the sampling distributions will converge to the optimal peak when $\alpha \geq 0.23$. Figure 8 reveals that a small perturbation of α has a very small effect on $F6$, but Figure 10 clearly indicates that the effect on the sampling distribution sequence is dramatic. These results confirm

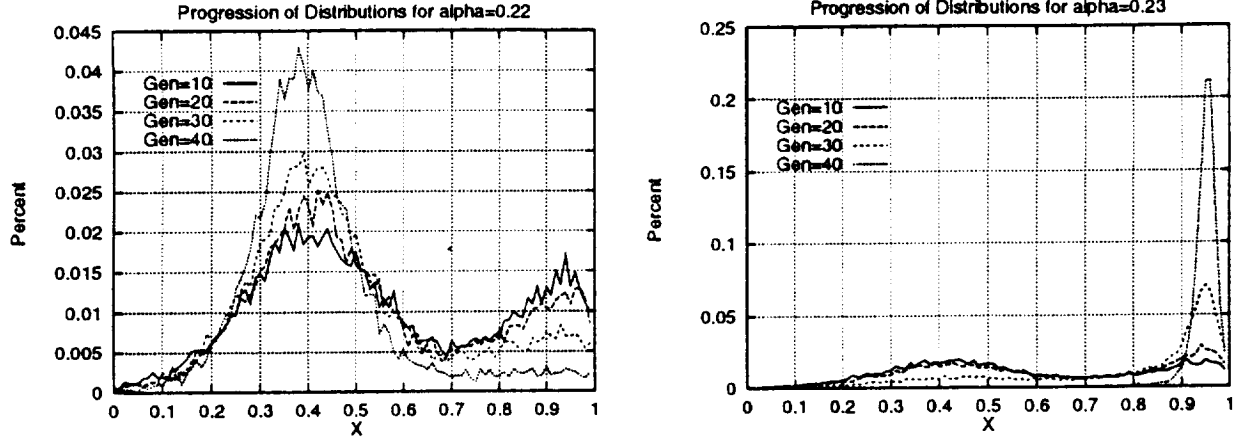


Figure 10: Sampling distributions generated by $F6$: *left*) when $\alpha = 0.22$, convergence is to the sub-optimal peak; *right*) when $\alpha = 0.23$, convergence is to the optimal peak.

the unstable, tug-of-war behavior of genetic algorithms on this function. More importantly, however, these results confirm that genetic algorithms can be *expected* to converge to sub-optima when applied to certain functions, even when the sampling of the objective function is adequate. Similar divergent behavior of canonical genetic algorithms has been observed on *deceptive* functions (Goldberg, 1987).

6.2 Critical Requirements

For Theorem 2 and its associated corollaries to be applicable, genetic algorithms must be representable in a form consistent with generational methods. This can be achieved by setting

$$Q_k(z', dx) = \int_X p_k(dz'') Q_k(z', z'', dx),$$

where p_k is described by (17). Thus, the genetic algorithm sampling distributions $\{P_{k+1}\}$ may be expressed according to (16).

If assumption (p) of Section 3.3 were replaced with

p'. the transition probabilities $Q_k(x', x'', \cdot)$ are defined by

$$\begin{aligned} Q_k(x', x'', A) = & \int_X 1_{\{z \in A, f_k(x') \leq f_k(z)\}} T_k(x', x'', dz) + \\ & 1_A(x') \int_X 1_{\{f_k(z) < f_k(x')\}} T_k(x', x'', dz), \end{aligned} \quad (53)$$

where $T_k(x', x'', dz)$ are transition probabilities,

it would only be necessary to prove that the transition probabilities, $T_k(x', x'', dz)$, weakly converge to $\varepsilon_{x'}(dz)$ for $k \rightarrow \infty$ and for all $x' \in \mathcal{X}$ to satisfy the requirements of Corollary 3. To prove this, however, would require additional assumptions on the objective function f .

To meet the requirements of Corollary 4, satisfaction of the following assumption would be sufficient.

r'. the transition probabilities $Q_k(x', x'', dz)$ are defined by

$$Q_k(x', x'', dz) = c_k(x') \varphi((z - x')/\beta_k) \mu_n(dz), \quad (54)$$

where φ is a continuous symmetrical finite density in \mathfrak{R}^n ,

$$\beta_k > 0, \quad \sum_{k=1}^{\infty} \beta_k < \infty, \quad c_k(x) = \frac{1}{\int_{\mathcal{X}} \varphi((z - x)/\beta_k) \mu_n(dz)};$$

The novel recombination operator described by (52) may be expressed in the form of (54) with $\beta_k = \alpha|x' - x''|$. To verify the satisfaction of this assumption, it must be proved that

$$\sum_{k=1}^{\infty} \beta_k < \infty.$$

The reason why this is not generally possible is discussed in subsection 6.1.

6.3 Ensuring Convergence to a Global Optimum

In the previous subsection, the missing links in applying Zhigljavsky's convergence proofs to genetic algorithms were revealed. In both cases, the critical requirement is proving that the distributions Q_k weakly converge sufficiently quickly to a probability measure concentrated at a point.

Rather than proving this property, it is possible to simply redesign the sampling distributions Q_k to ensure this property is satisfied. Consider the following assumption:

r''. the transition probabilities $Q_k(x', x'', dz)$ are defined by

$$Q_k(x', x'', dz) = c_k(x') \varphi((z - x')/\beta_k) \mu_n(dz), \quad (55)$$

where φ is a continuous symmetrical finite density in \mathfrak{R}^n ,

$$\beta_k = \min\{\alpha|x' - x''|, \gamma_k\}, \quad (56)$$

$$x' \neq x'', \quad c_k(x) = \frac{1}{\int_{\mathcal{X}} \varphi((z - x)/\beta_k) \mu_n(dz)},$$

and

$$\gamma_k > 0, \quad \sum_{k=1}^{\infty} \gamma_k < \infty.$$

Selecting β_k as in (56) allows the continued exploitation of similarities for adaptation and improved efficiency, and it forces the reduction of local search breadth at a sufficient rate to prevent diffusion of the sampling distribution away from global optima. To allow for nearly normal genetic algorithm performance, a conservative γ_k schedule, which satisfies (r''), could be used.

Using the assumptions in Appendix B, the assumption that the feasible space, \mathcal{X} , is a compact metric space of arbitrary type, and assumptions (p') and (r'') above permit the following corollaries.

Corollary 6 *Let the conditions (c), (d), (e), (h), (i), (j), (o), (q), (t), and (p') be satisfied. Furthermore, let (r'') be satisfied for the transition probabilities $T_k(x', x'', dz)$ of (53). Then the sequence of distributions determined by (21) weakly converges to $\varepsilon^*(dx)$ for $k \rightarrow \infty$.*

Proof: All of the conditions of Corollary 3 are satisfied. ■

Corollary 7 *Let the conditions (e), (h), (i), (j), (q), (t), and (r'') be satisfied. Then the sequence of distributions determined by (21) weakly converges to $\varepsilon^*(dx)$ for $k \rightarrow \infty$.*

Proof: All of the conditions of Corollary 4 are satisfied. ■

Corollaries 6 and 7 demonstrate that genetic algorithms can be constructed in a manner to ensure convergence to a global optimum.

Interestingly, even when very small values of α where used in (51), a genetic algorithm using forced local search reduction (FLSR) applied to the distribution in (52) consistently

converged to the global optimum. FLSR has also been applied to other novel recombination operators and shown to be highly effective when optimizing the functions in De Jong's test suite (Peck, 1993).

7 Conclusions

In this paper, the theory of global random search methods is applied to genetic algorithms, and genetic algorithms are generalized into a broader class of methods. This broader class includes those global random search methods with probability transition operators that are dependent on two globally obtained samples.

A primary tenet of this paper is that the construction and evolution of the sampling distributions $\{P_{k+1}\}$, particularly in the context of the phenospace, is the preferred basis for understanding genetic algorithm behavior. It is the preferred basis because it operates at the level of abstraction most appropriate for understanding the interplay among the search of the objective function, the procedural elements, and generating mechanisms of the genetic algorithm. Accordingly, the genetic algorithm is reformulated in terms of sampling distributions and generalized in terms of the phenospace. Three heuristics to aid in the understanding of genetic algorithm design and behavior are also introduced.

The factors affecting these sampling distributions are considered extensively. It is concluded that: there are many advantages to exploiting candidate solution similarities directly, selection variance can be expected to degrade performance, the best traditional recombination operators have localized search distributions that are increasingly constrained in breadth as the distance between the parents decreases, genetic algorithms are robust with respect to initial populations, and FIFO deletion is more exploitative than generational replacement.

Sufficient conditions for convergence to a global optimum are also established. These conditions ensure that the transition probabilities, which are otherwise constrained primarily by the similarities of two globally obtained and possibly dissimilar samples, are adequately localized. These sufficient conditions for convergence, however, are purchased at the cost of

one of the most appealing characteristics of genetic algorithms: its totally adaptive nature. To theoretically ensure weak convergence to a global optimum, a schedule for constraining the search breadth of the recombination operator must be supplied.

There are many opportunities for further research related to this paper: deriving the relationship between high sampling variance and poorer selection performance, reducing selection sampling variance in sequential or steady-state methods, reexamining the population sizing problem to make the dependencies on the complexity of \mathcal{X} and f explicit, weakening the sufficient conditions for the weak convergence of genetic algorithms to a global optimum, and developing a fully adaptive method that is provably convergent, but does not depend on scheduled control of the transition probabilities.

A Weak Convergence

In this appendix, weak convergence is defined. The presentation is adapted from (Billingsley, 1971).

Let \mathcal{X} be a separable and complete metric space. Denote the interior, closure, and boundary of a set S as S° , S^- , and ∂S , respectively, where ∂S is $S^- - S^\circ$. Denote the class of bounded, continuous real-valued functions on \mathcal{X} as $C(\mathcal{X})$. Let the σ -algebra generated by the open sets in \mathcal{X} be denoted \mathcal{B} , and note that all functions in $C(\mathcal{X})$ are measurable with respect to \mathcal{B} .

Weak convergence is concerned with the nonnegative, completely additive set functions P on \mathcal{B} for which $P(\mathcal{X}) = 1$ (*i.e.*, probability measures). A set S whose boundary satisfies $P(\partial S) = 0$ is referred to as a P -continuity set. If P_k and P are probability measures on $(\mathcal{X}, \mathcal{B})$, then P_k converges weakly to P , denoted $P_k \Rightarrow P$, if

$$\lim_{k \rightarrow \infty} \int_{\mathcal{X}} f dP_k = \int_{\mathcal{X}} f dP \quad (57)$$

for all functions f in $C(\mathcal{X})$ (Billingsley, 1971). The convergence of integrals of functions forms the basis of this definition of weak convergence. Weak convergence may also be characterized in terms of the convergence of the measures of sets.

Theorem 4 *These conditions are equivalent:*

- a. $P_k \Rightarrow P$,
- b. $\limsup_k P_k(F) \leq P(F)$ for all closed F ,
- c. $\liminf_k P_k(G) \geq P(G)$ for all open G ,
- d. $\lim_k P_k(S) = P(S)$ for all P -continuity sets S .

Proof. A proof is provided in (Billingsley, 1971, Thm. 2.1).

B Assumptions

The following list comprises the assumptions used in this paper. These assumptions and the following commentary are adapted from (Zhigljavsky, 1991, §5.2.1).

- a. $\xi_k(x)$ for any $x \in \mathcal{X}$ and $k = 1, 2, \dots$ are random variables having a zero-mean distribution $F_k(x, d\xi)$ concentrated on a finite interval $[-d, d]$; and the random variables $\xi_{k_1}(x_1), \xi_{k_2}(x_2), \dots$ are mutually independent for any k_1, k_2, \dots and x_1, x_2, \dots from \mathcal{X} ;
- b. $y_k(x) = f_k(x) + \xi_k(x) \geq c_1 > 0$ with probability one for all $x \in \mathcal{X}, k = 1, 2, \dots$;
- c. $0 < c_1 \leq f_k(x) \leq M_k = \sup f_k(x) \leq C < \infty$ for all $x \in \mathcal{X}, k = 1, 2, \dots$;
- d. the sequence of functions $f_k(x)$ converges to $f(x)$ for $k \rightarrow \infty$ uniformly in x ;
- e. $Q_k(z, dx) = q_k(z, x)\mu(dx)$,

$$\sup_{z, x \in \mathcal{X}} q_k(z, x) \leq L_k < \infty$$

for all $k = 1, 2, \dots$ where μ is a probability measure on $(\mathcal{X}, \mathcal{B})$;

- f. the random elements χ_1, \dots, χ_N with a distribution $R(dx_1, \dots, dx_N)$ defined on $\mathcal{B}_N = \sigma(\mathcal{X} \times \dots \times \mathcal{X})$ are symmetrically dependent⁴. That is, for any choice of distinct positive integers i_1, \dots, i_N , the joint distribution of

$$\chi_{i_1}, \dots, \chi_{i_N}$$

depends only on N and is independent of the integers i_1, \dots, i_N (Blum, Chernoff, Rosenblatt & Teicher, 1959);

- g. the probability distribution $P_M(dx_1, \dots, dx_M)$ on \mathcal{B}_M is described in terms of the distribution $R_N(dx_1, \dots, dx_N)$ through

$$P_M(dx_1, \dots, dx_M) = \int_{Z^N} \Pi(d\Theta_N) \prod_{j=1}^M \Psi(\Theta_N) \sum_{i=1}^N \Lambda(z_i, \xi_i, dx_j), \quad (58)$$

where

$$\begin{aligned} \Theta_N &= \{z_1, \dots, z_N, \xi_1, \dots, \xi_N\}, \\ Z &= \mathcal{X} \times [-d, d], \\ \Pi(d\Theta_N) &= R_N(dz_1, \dots, dz_N) F(z_1, d\xi_1) \dots F(z_N, d\xi_N), \\ \Psi(\Theta_N) &= \frac{1}{\sum_{j=1}^N (f(z_j) + \xi_j)}, \\ \Lambda(z, \xi, dx) &= (f(z) + \xi) Q(z, dx); \end{aligned}$$

- h. the global maximizer x^* of f is unique, and there exists $\varepsilon > 0$ such that f is continuous in the set $B(x^*, \varepsilon) = B(\varepsilon)$;
- i. μ is a probability measure on $(\mathcal{X}, \mathcal{B})$ such that $\mu(B(\varepsilon)) > 0$ for any $\varepsilon > 0$;
- j. there exists $\varepsilon_0 > 0$ such that the sets $A(\varepsilon) = \{x \in \mathcal{X} : f(x^*) - f(x) \leq \varepsilon\}$ are connected for any $\varepsilon, 0 < \varepsilon \leq \varepsilon_0$;

⁴Symmetrically dependent random variables are also called *interchangeable* (Blum, Chernoff, Rosenblatt & Teicher, 1959) and *exchangeable* (Loève, 1963).

- k. the sequence of probability measures $Q_k(x, dz)$ weakly converges to $\varepsilon_x(dx)$, for any $x \in \mathcal{X}$ as $k \rightarrow \infty$, where $\varepsilon_x(dx)$ is the probability measure concentrated at the point x ;
- l. the sequence of probability measures $R(k, N_k, x; dz)$ weakly converges to $\varepsilon_x(dx)$, for any $x \in \mathcal{X}$ as $k \rightarrow \infty$;
- m. for any $\varepsilon > 0$ there are $\delta > 0$ and a natural k_0 such that $P_k(B(\varepsilon)) \geq \delta$ for all $k \geq k_0$;
- n. for any $\varepsilon > 0$ there are $\delta > 0$ and a natural k_0 such that $P(k, N_{k-1}; B(\varepsilon)) \geq \delta$ for all $k \geq k_0$;
- o. the functions f_k , for $k = 1, 2, \dots$ are evaluated without random noise;
- p. the transition probabilities $Q_k(x, \cdot)$ are defined by

$$Q_k(x, A) = \int_{\mathcal{X}} 1_{[z \in A, f_k(x) \leq f_k(z)]} T_k(x, dz) + 1_A(x) \int_{\mathcal{X}} 1_{[f_k(z) < f_k(x)]} T_k(x, dz), \quad (59)$$

where $T_k(x, dz)$ are transition probabilities, weakly converging to $\varepsilon_x(dz)$ for $k \rightarrow \infty$ and for all $x \in \mathcal{X}$;

- q. $P_1(B(x, \varepsilon)) > 0$ for all $\varepsilon > 0$, $x \in \mathcal{X}$;
- r. the transition probabilities $Q_k(x, dz)$ are defined by

$$Q_k(x, dz) = c_k(x) \varphi((z - x)/\beta_k) \mu_n(dz), \quad (60)$$

where φ is a continuous symmetrical finite density in \mathbb{R}^n ,

$$\beta_k > 0, \quad \sum_{k=1}^{\infty} \beta_k < \infty, \quad c_k(x) = \frac{1}{\int_{\mathcal{X}} \varphi((z - x)/\beta_k) \mu_n(dz)};$$

- s. $f_k(x) = f(x)$, $\xi_k(x) = \xi(x)$, $Q_k(x, dz) = Q(x, dz)$ for each $k = 1, 2, \dots$; and
- t. $f_k(x) = f(x)$ for $k = 1, 2, \dots$

A few of Zhigljavsky's comments regarding these assumptions will now be related.

Condition (a) makes two basic requirements on the evaluation noise: it must be independent, and it must be concentrated on a finite interval. The requirement of finiteness is particularly important. If the evaluation noise at a suboptimal point is positive and very large, then all subsequent evaluations will occur in its vicinity with large probability. This holds even if the search was already concentrated at the global maximizer.

The requirement of condition (b) may be easily satisfied by constructing an auxiliary function $\tilde{f}_k(x)$ from $f_k(x)$ such that (b) is satisfied. If an α_k is known such that $P\{\sup |\xi_k(x)| \leq \alpha_k\}$ is equal or almost equal to one, then a function $\tilde{f}_k(x)$ based on $f_k(x)$ that can be made arbitrarily close to $\max\{c_1, f_k(x) + \text{constant}\}$ is presented in (Zhigljavsky, 1991).

The conditions (h), (i), and (j) are natural and non-restrictive (Zhigljavsky, 1991). The uniqueness requirement of the global maximizer x^* is imposed to simplify some formulations. Zhigljavsky notes that the results presented actually deal with distribution convergence to a distribution concentrated on the set

$$\bigcap_{\varepsilon > 0} A(\varepsilon) \supset \{\arg \max f(x)\} \quad (61)$$

instead of convergence to $\varepsilon_{x^*}(dx)$. Therefore, the uniqueness requirement can be relaxed, and convergence can be understood in this sense. Condition (j), when imposed, does require that the set (61) be connected.

Necessary requirements on the parameters of Procedure 3 are formulated in conditions (e), (k), and (l). Distributions satisfying these requirements, however, are very easily constructed.

The assumptions formulated in (f), (g), and (s) are not requirements. They are only auxiliary tools for formulating Lemma 1. In this formulation, Θ_N is an N -fold sampling of \mathcal{X} and the noise process (*i.e.*, $\Theta_N \in Z^N$). The probability of sampling a subregion of Z^N is described by the distribution $\Pi(d\Theta_N)$. The sampling distribution for a particular dx is described by

$$\Psi(\Theta_N) \sum_{i=1}^N \Lambda(z_i, \xi_i, dx) = \sum_{i=1}^N \frac{f(z_i) + \xi_i}{\sum_{j=1}^N (f(z_j) + \xi_j)} Q(z_i, dx),$$

which is analogous to (16) in Procedure 3.

Assumptions (m) and (n) may be regarded as conditions imposed on the parameters of Procedure 3. Since these conditions are not constructive, easily verifiable conditions sufficient for the validity of (m) or (n) are of interest (Zhigljavsky, 1991). The conditions (p), (q), and (r) represent such sufficient conditions for two widely used forms of transition probabilities. A realization y_k from (59) may be obtained by sampling the distribution $T_k(x, \cdot)$ to get ζ_k and setting

$$y_k = \begin{cases} \zeta_k & \text{if } f_k(\zeta_k) \geq f_k(x) \\ x & \text{otherwise.} \end{cases}$$

This form of transition probability is suitable only when the functions f_k are evaluated without noise. When noise is present, (60) is a natural way of determining transition probabilities for $\mathcal{X} \subset \mathbb{R}^n$. A random realization y_k in \mathcal{X} from the distribution $Q_k(x, \cdot)$ in (60) may be obtained by repeatedly sampling φ to obtain a realization ζ_k until $x + \zeta_k \in \mathcal{X}$, then setting $y_k = x + \zeta_k$. When $\mathcal{X} \subset \mathbb{R}^n$, the transition probabilities of $T_k(x, \cdot)$ of (59) may be chosen using (60).

Zhigljavsky finally observes that condition (q) places requirements on both \mathcal{X} and P_1 . When $\mathcal{X} \subset \mathbb{R}^n$ and \mathcal{X} is of non-zero Lebesgue measure, then (q) means that the P_1 -measure of any non-empty ball in \mathbb{R}^n with the center in \mathcal{X} is larger than zero and that \mathcal{X} has no *appendices*⁵.

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⁵Appendices are those parts for which there exist non-empty balls in \mathbb{R}^n having centers in these parts and with zero Lebesgue measure of the intersection of these balls and \mathcal{X} .

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